

OPTIMIZATION OF SUPPLY CHAIN MANAGEMENT
AND FACILITY LOCATION SELECTION FOR A BIOREFINERY

A Thesis

by

IAN MICHAEL BOWLING

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

December 2010

Major Subject: Chemical Engineering

Optimization of Supply Chain Management and Facility Location Selection for a
Biorefinery

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Approved by:

Chair of Committee,	Mahmoud M. El-Halwagi
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ABSTRACT

Optimization of Supply Chain Management and Facility Location Selection for a
Biorefinery. (December 2010)

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Chair of Advisory Committee: Dr. Mahmoud M. El-Halwagi

If renewable energy and biofuels are to attain success in the market place, each step of their production and the system as a whole must be optimized to increase material and energy efficiency, reduce production cost and create a competitive alternative to fossil fuels. Systems optimization techniques may be applied to product selection, process design and integration, feedstock procurement and supply chain management to improve performance. This work addresses two problems facing a biorefinery: technology selection and feedstock scheduling in the face of varying feedstock supply and cost. Also addressed is the optimization of a biorefinery supply chain with respect to distributed processing of biomass to bio-products via preprocessing hubs versus centralized processing and facility location selection. Two formulations are proposed that present a systematic approach to address each problem. Case studies are included to demonstrate model capabilities for both formulations. The scheduling model results display model sensitivity to feedstock price and transport distance penalized through carbon dioxide emissions. The distributed model shows that hubs may be used to extend the operating radius of a biorefinery and thereby increase profits.

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Dr. El-Halwagi's patient instruction and support made this work possible. I am so grateful for his leadership. Beyond instruction in the application of systems optimization to process design problems, he allowed my mind to wander to address issues that interested me and offered guidance to bring about their successful completion. I would also like to thank the members of my committee Dr. Baldwin and Dr. Barrufet for their support.

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1. INTRODUCTION: MOTIVATION

Renewable energy and biofuels have received an increased share of attention in recent years. Concerns over the long-term sustainability of fossil fuels, global climate change, the rising cost of transportation fuel, and energy independence have all been proposed as reasons for increasing the use of renewable energy sources in the United States. At the very least, if renewable energy is the future, it is preferred to be on the leading edge of the technology and experience curve.

1.1 Sustainability

Sustainability has been defined as; “meeting the needs of the present without compromising the ability of future generations to meet their own needs” (UN, 1987). When compared with this standard, consumption of petroleum derived energy is not sustainable. The extraction and use of oil today depletes a resource of finite quantity. As the world supply of crude becomes increasingly scarce in the future, the cost of energy may increase to a point of becoming prohibitively expensive. If alternatives capable of meeting world demand have not been developed an energy crisis may be the result. Development of renewable and sustainable alternatives today to meet a fraction of our energy needs will slow the depletion of petroleum resources and allow future generations to better leverage renewable energy technologies if they must be relied upon completely.

Experience in the production, distribution and use of renewable energy may be developed now while stakes are low and the penalty for failure is not catastrophic to the economy or standards of living.

As shown in Figures 1 and 2 as worldwide energy consumption increases global production of crude oil has increased to meet rising demand. New production technology has made previously unrecoverable petroleum profitable and new areas are found to contain fossil fuels, which has increased the world level of proven petroleum reserves. However, improving extraction methods and new reserves do not detract from the previous thoughts on long-term sustainability. The accelerating extraction of oil may increase one's concern for the long term sustainability of petroleum-derived products.

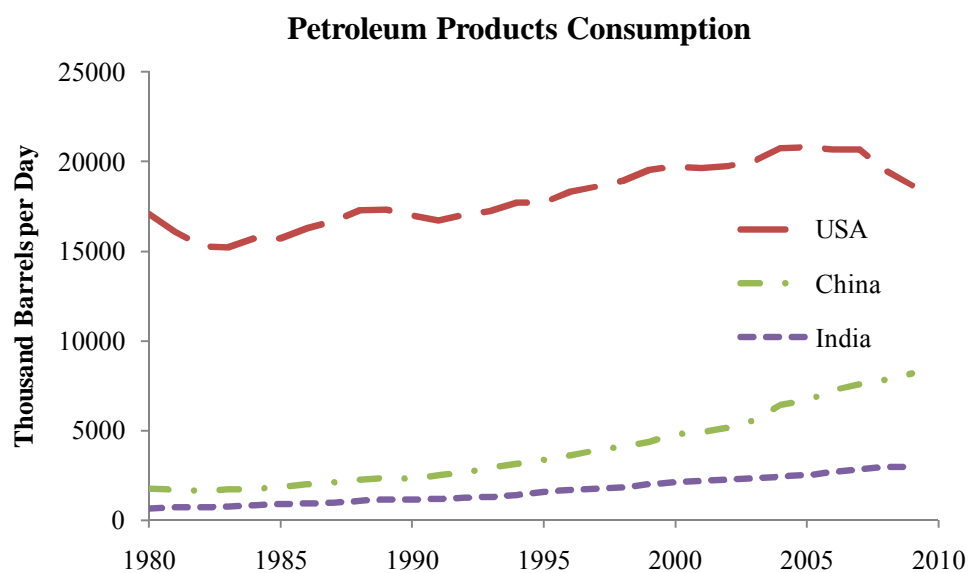


Figure 1. Petroleum Products Consumption, Selected Nations

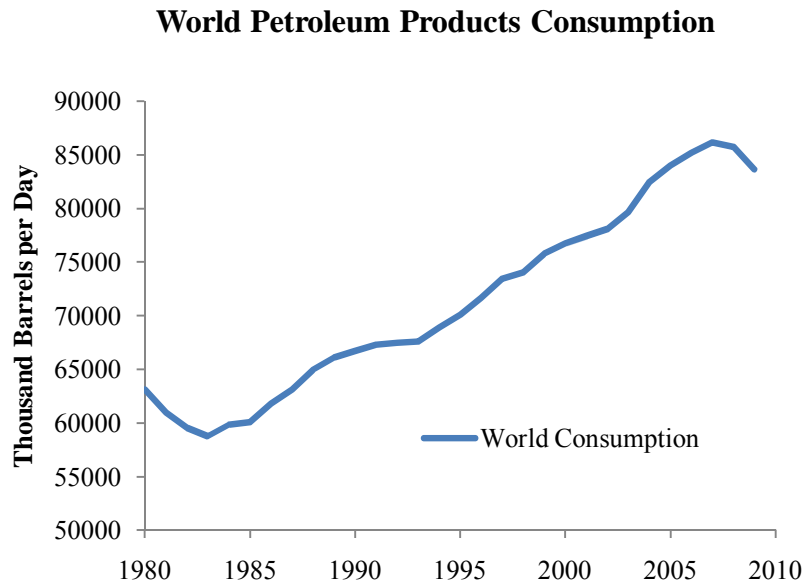


Figure 2. World Petroleum Products Consumption

1.2 Global Climate Change

Global climate change and its potential link with anthropogenic carbon emissions have also created a drive to adopt renewable energy sources that are more environmentally friendly. The increasing use of carbon dioxide emitting energy in developing nations will only continue to drive emission rates further upward (See Figures 3, 4 and 5). Second generation biofuels that are carbon neutral across their lifecycle are of particular interest, as they do not contribute more carbon dioxide to the atmosphere than they removed from it during their growth. Additionally, research has occurred in the area of carbon-negative biofuels where after processing a bio-char is returned to the soil as a carbon sequestration method (Mathews, 2008; Zhou et. al., 2009; Tillman et. al., 2006).

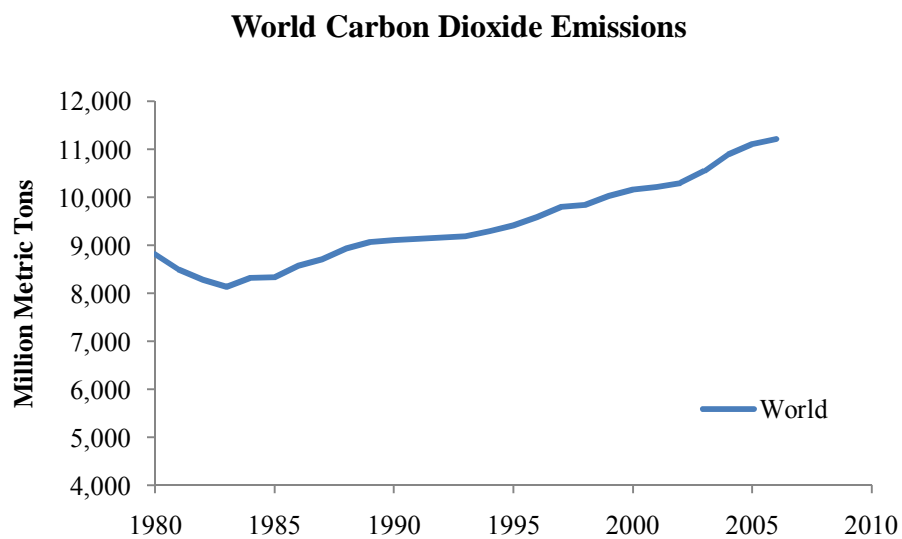


Figure 3. Global Carbon Dioxide Emissions

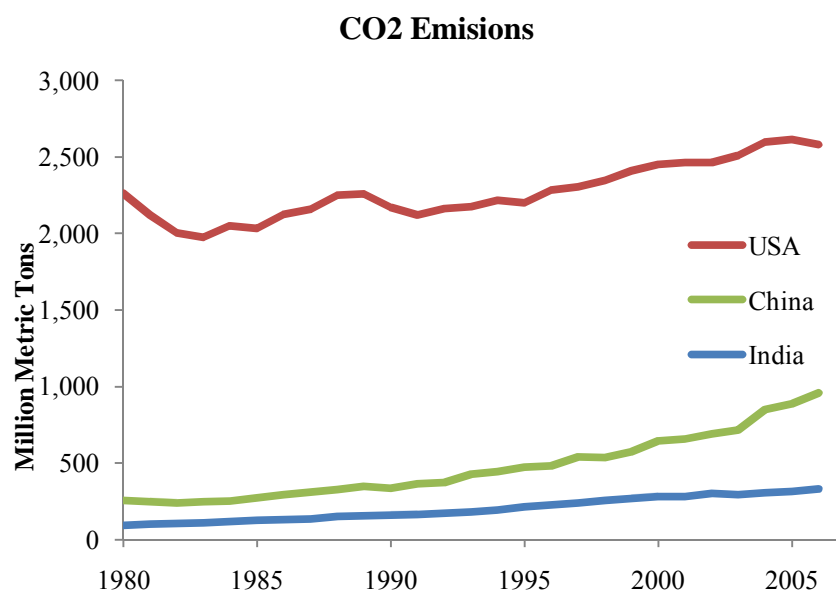


Figure 4. Carbon Dioxide Emissions, Selected Countries

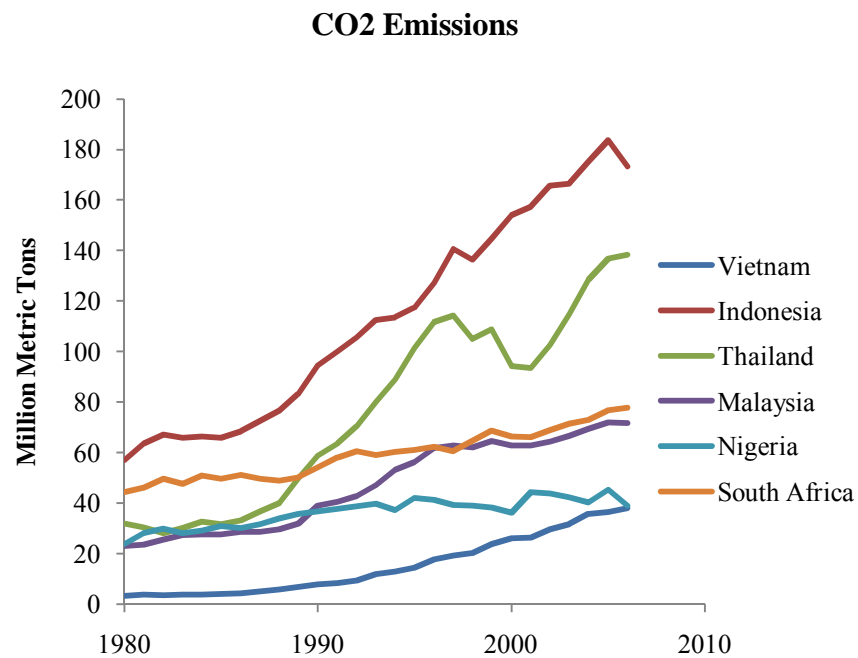


Figure 5. Carbon Dioxide Emissions, Emerging Countries

1.3 Cost of Transportation Fuels

The rising price of transportation fuels was a topic covered extensively during the 2008 presidential election in the United States. Data from the Consumer Expenditure Survey in Figure 6 shows that on average, Americans are spending a higher fraction of their total earned income on gasoline and motor oil (Bureau of Labor and Statistics, 2010).

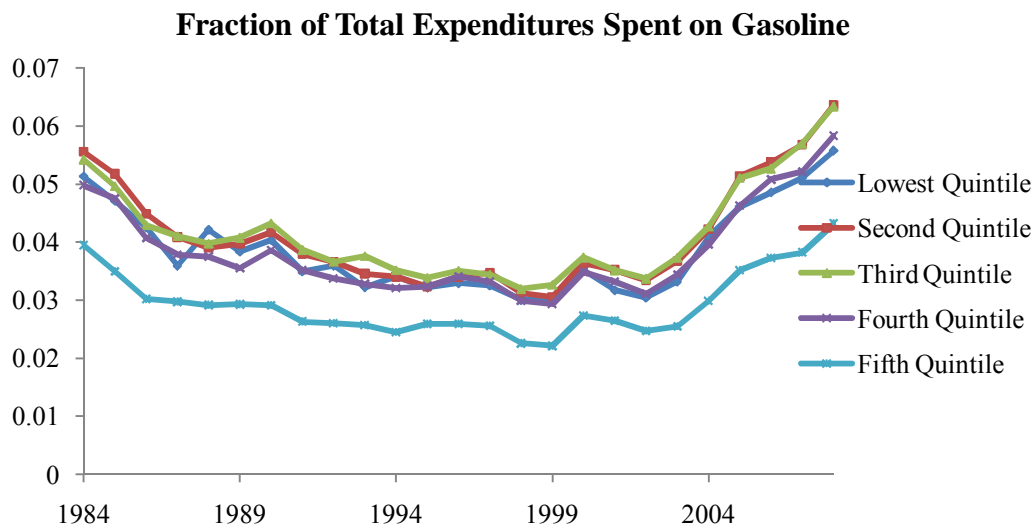


Figure 6. Fraction of Income Spent on Fuel in United States

1.4 Energy Security and Domestic Biomass

China and India account for a share of the increasing global energy use. As both populous nations become increasingly industrialized and work to raise standards of living their energy consumption also increases. Both nations, like the United States, are also net energy importers. China is the second largest oil consumer (EIA, 2010) and India, which imports roughly seventy percent of its oil, is the fourth largest consumer of petroleum products in the world (EIA, 2010b). A report issued by the International Energy Agency in July 2010 calculates that China has overtaken the United States as the world's largest energy consumer (EIA, 2010c). Economic competition for energy is a potential source of conflict between nations, particularly as petroleum reserves decline and prices increase.

Energy security has been used as another reason necessitating the use of domestically produced renewable energy sources. Its importance to the general public as a source of concern was reflected in its prominence as a major issue in the 2008 presidential election campaigns. Much of the research in the area of biofuels is funded through Defense Advanced Research Projects Agency (DARPA) in an effort to reduce the US military's dependence on foreign petroleum to power aircraft, vehicles and ships (DARPA, 2010). Several studies have been conducted to review the impact of the price of energy on the US economy. (Cunado and Gracia, 2005; Hunt et. al., 2002; Leduc and Sill, 2004) Higher energy prices can suppress economic growth by increasing the cost of other commodities affecting core inflation. This link can be seen in the changes in Gross Domestic Product growth following dramatic fluctuations in the world oil price shown in Figure 7. Price shocks in 1973 and 1974, the late 1970s and early 1980s, the early 1990s and in 2008 were followed by economic recessions (EIA, 2010d).

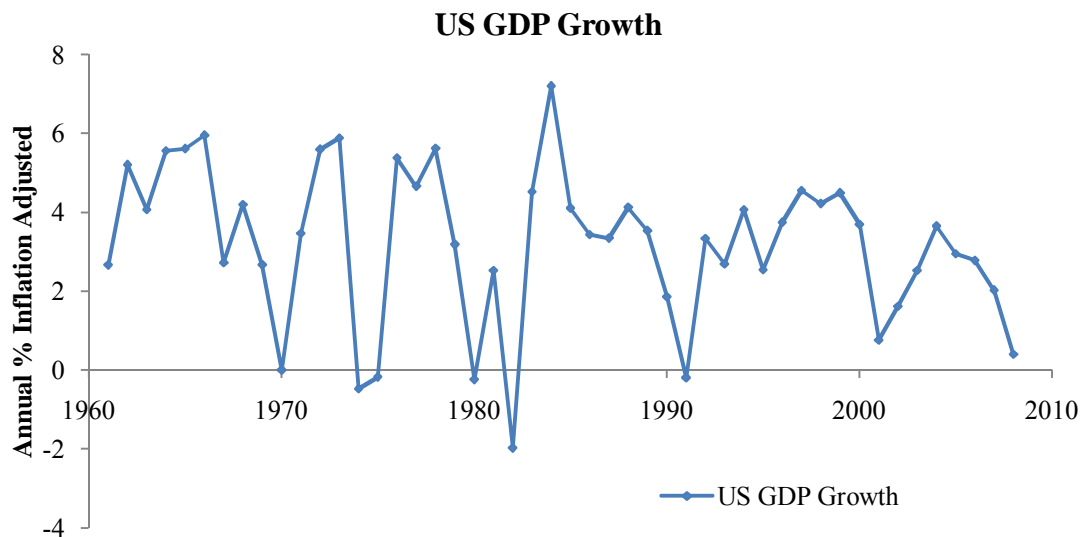


Figure 7. United States Gross Domestic Product Growth (World Bank, 2010)

1.5 Government Incentives for Biofuels

In early 2010 the United States President announced several initiatives geared towards encouraging the use of renewable liquid fuels in the US to “enhance American energy independence while building a foundation for a new clean energy economy.” Steps include a long-term renewable fuels mandate of 36 billion gallons by 2022 established by Congress (DOE, 2010). Also, for the first time in order to comply with the rule, some renewable fuels must achieve greenhouse gas emissions reductions when compared to the petroleum derived gasoline or diesel they displace.

The Biomass Crop Assistance Program proposed by the USDA will provide grants, loans, and other financial support to encourage the use of biomass for biofuels and other bio-derived chemical products. The goal of this program is to speed up the

commercialization of developing biomass to bio-products technologies. Assistance with the collection, harvesting, storage and transportation costs of eligible biomass will be given (USDA, 2010).

The President also formed a Biofuels Interagency Working Group comprised of individuals from the Department of Energy, US Department of Agriculture and the Environmental Protection Agency to develop a comprehensive strategy for investing in renewable energy and reducing the nation's dependence upon foreign oil.

Presently the US government shows support for biodiesel and renewable diesel in the form of a \$1.00/gallon production tax credit (IRS, 2010). This tax credit expired in 2010, but was recently reinstated retroactively for 2010 (REW, 2010). Many states, including Texas, also have a tax exemption on biomass derived diesel fuels.

Diesel fuel tax exception. The tax imposed on the first sale or use of diesel fuel in this state does not apply to biodiesel or to the volume of water, fuel ethanol, or biodiesel that is blended with taxable diesel fuel, when the finished product is clearly identified on the retail pump, storage tank, and sales invoice as biodiesel or a combination of diesel fuel and water, fuel ethanol, or biodiesel. Texas Administrative Code (Tax Code, §§162.003, 162.204, and 162.227)

These subsidies and tax exemptions are important for biodiesel manufacturers to be able to produce fuel at a cost that is reasonably comparable to petroleum-derived fuels.

The recent decline in oil prices associated with the economic downturn beginning in 2009 may cause many of these energy related issues to lose steam in the political arena, however as the global economy recovers and the fundamental issues remain unchanged, how we obtain the energy required to fuel our economy will resurface as a topic of importance.

1.6 Summation

There are many reasons to work towards the adoption of renewable energy and biofuels in particular. Leaving future generations with the advantages of reasonably priced sources of energy for their use, moderating the increasing cost of transportation fuels as supply grows tighter in a more competitive global energy market, protecting the environment by developing cleaner fuels or insuring the availability of energy to fuel economic development for our nation might all be posed as reasons for increasing renewable energy's role in the nation's energy mix. However, if renewable sources of energy are to move beyond a niche market and into a larger role in the market place they must be able to compete against traditional fossil fuels. Process optimization must be done at every level of the value chain from the field to the gasoline pump. Systems optimization can contribute to renewable biofuels viability by moving beyond the myopic view of only unit operation based optimization and look across the entire life cycle from field to tank for process improvements and synergy. Systematic optimization techniques have already been applied successfully to optimal pathway selection, partnering different conversion methods to increase overall yields, scheduling and

transportation optimization, material efficiency, waste minimization and energy conservation.

2. BIOMASS TO BIOFUEL PATHWAYS

2.1 Pyrolysis

Pyrolysis is the thermochemical process that converts biomass into a liquid bio-crude, charcoal and non-condensable gases, acetic acid, acetone and methanol by heating the biomass to 650-800 K in the absence of air. Pyrolysis produces energy fuels with high fuel-to-feed ratios, and the product slate can be modified by adjusting the operating temperature and pressure within the reactor. Goyal et. al. (2008) conducted a review of thermal conversion of biomass to biofuels with an emphasis on pyrolysis and the product distributions at different operating conditions for varied feedstocks. Demirbas (2001b) also published a review of the biomass to bio-product conversion processes available and suggested the potential for wood residual from saw-mills be used to produce energy and valued chemical products.

2.2 Liquefaction

Liquefaction is a low temperature (525-600K), high pressure (5-20MPa) reaction in the presence of a catalyst in which feedstock macro-molecule compounds are decomposed into fragments of light molecules which then repolymerize into oily compounds of higher molecular weight (Demirbas, 2000). Liu and Zhang (2008) observed the effects of various solvents on the biomass liquefaction process while seeking to optimize around the production of fuel additives and valued chemicals and found ethanol and acetone to be the most promising solvents. Xu and Etcheverry (2008) investigated liquefaction of biomass with and without iron-based catalysts in sub and

super critical solutions of ethanol and concluded that the catalyst increased oil yields. The effect of lignin content on liquefaction products was observed by Demirbas (2001b) the presence of low molecular weight phenolic compounds were seen to decrease with decreasing lignin content.

2.3 Gasification

Gasification converts biomass to syn-gas, a combustible gas mixture primarily consisting of methane, carbon monoxide and hydrogen. Like pyrolysis, biomass is heated in the absence of oxygen, however the operating temperatures used are typically higher on the order of 1100-1200K. McKendry (2001) investigated biomass gasification to generate fuel to supplement landfill gases that could be used for electric power generation. The work also included an economic comparison of waste biomass versus biomass grown specifically for conversion to energy. Valero and Uson (2006) developed operation maps for oxy-gasification of biomass and coal to relate key gasification parameters to available operator degrees of freedom to assist in optimizing gasifier performance and decrease unit malfunctions. Research has also focused on wet biomass gasification to illuminate the need for feedstock drying prior to gasification (Kruse, 2009). The product syn-gas may also be used as a starting point for producing higher valued chemicals like transportation fuels (Durham, 2010; Hamelinck et. al., 2004; Tavasoli et. al., 2006), methanol (Hamelinck et. al. 2002) di-methyl ether (Naqvi, 2010; Arcoumanis et. al., 2008; Semelsberger et. al., 2006), and hydrogen (Lu et. al., 2007; Specht et. al., 1998; Cifre and Badr, 2007).

2.4 Biochemical Conversion Pathways

Anaerobic digestion of biomass occurs via bacteria in the absence of oxygen and produces a mixture of methane and carbon dioxide called biogas (Santosh et. al., 2004; Ranade et. al., 1987; Berglund and Borjesson, 2006). Alcoholic Fermentation is one type of anaerobic fermentation in which alcohols are produced from sugars found in biomass by enzymatic hydrolysis of sucrose followed by fermentation of simple sugars (Fischer et. al., 2008; Yazdani and Gonzalez, 2007; Elshahed, 2010).

2.5 Biodiesel

Biodiesel is the conversion of triglycerides found in vegetable oils to fatty-acid methyl-esters (FAME). Myint and El-Halwagi (2009) applied process integration and systems optimization techniques to the biodiesel process to increase material and energy efficiency while improving process economics and reducing the environmental burden. Capital cost estimation for the integrated flowsheet was then conducted in addition to economic analysis including the impact of soybean oil price on overall process profitability.

Pokoo-Aikens et. al. (2010a) investigated the use of algal oil produced via carbon capture from flue gas as feedstock for biodiesel. Economic analysis showed that with successful process integration, an optimized algae to oil process and favorable markets for product biodiesel and glycerol could make the process a competitive alternative to edible feedstocks. Pokoo-Aikens et. al. (2010b) later included safety metrics in a multi-criteria analysis of various alternative feedstocks and technologies for biodiesel including animal fats, waste oils and lipids found in sewage sludge. Economic

comparison of solvents used for oil extraction pointed towards the use of hexane and toluene, while the safety analysis rated methanol and ethanol more highly. The trade-off between cost and safety was then discussed.

Hydrogenation derived renewable diesel (HDRD), the product formed when vegetable oils are hydrotreated over metallic catalysts, has also been investigated as a potential way to integrate plant oils into traditional crude oil refineries (Stumborg et. al., 1996; Knothe, 2009; Huber, 2007). Donnis et. al. (2009) described the chemical reaction kinetics in detail and proposed a rate mechanism using two reaction pathways, decarboxylation in which oxygen is removed as carbon oxides and hydrogenation which removes oxygen as water. The decarboxylation route, while consuming less hydrogen leads to a reduction in product formation as some carbon leaves as a waste stream. A measure of control over pathway selection was thought to be given by manipulating reaction pressure.

3. SYSTEMS OPTIMIZATION AND BIOFUELS

3.1 Biorefinery Optimization

Systems optimization techniques have been focused on several aspects of biorefining including; selecting the appropriate process configuration or product slate, integration of varied technologies or feedstocks, optimal facility capacity selection, and supply chain optimization including maximum feedstock supply range and mode of transportation. Mohan and El-Halwagi (2007) developed a systematic algebraic procedure for targeting cogeneration opportunities utilizing biowaste or biomass ahead of power generation network design. The work used process integration strategies with cascade techniques to reconcile thermal demands and power generation opportunities. The work also discussed the importance of green house gas pricing options to the overall economic assessment of the process. Aksoy et. al. (2008) proposed the use of poultry litter, presently an environmental burden, as a feedstock for generating heat, power and other valued chemicals at a biorefinery. Optimization techniques were used to determine the best large scale biorefinery capacity and optimal location given three levels of litter availability. Sammons et al. (2008) incorporated economic perspective along with modeling and simulation insight to analyze an integrated biorefinery and develop a systematic framework that evaluates environmental and economic measures for the optimization of process and product selection. Tan et al. (2009) developed an extended input-output model using fuzzy linear programming to determine the optimal capacities of distinct process units given a predefined product mix and environmental (carbon, land and water footprint) goals. Elms and El-Halwagi

(2010) introduced an optimization routine for feedstock selection and scheduling for biorefineries and included the impact of greenhouse gas policies on the biorefinery design. Ng et al. proposed a hierarchical procedure for the synthesis of potential pathways and developed a systematic approach to screen and identify promising pathways for integrated biorefineries. Alvarado-Morales (2009b) also proposed a systematic methodology to analyze and improve processing routes for conversion of biomass to biofuels, select which product to produce and which sequence of unit operations to apply to obtain the highest profit for the biorefinery. Besler et. al. (2009) proposed a mixed integer linear program capable of screening through a myriad of potential reaction pathways for conversion of biomass to biofuels with the objective of identifying potential process bottlenecks and promising pathways. Metabolic pathway analysis is used to generate multiple reaction pathways which are then screened on varying criteria until an optimal pathway is selected. While Searcy and Flynn (2010) proposed that the most socially relevant metric for technology selection is the minimum incremental cost per unit of greenhouse gas reduction.

Alvarado-Morales et al. (2009a) proposed an integrated process design and control problem to optimize the economic performance of a bioethanol facility considering reactor controllability and downstream purification energy requirements. There is also ongoing research to establish processing routes with minimum energy consumption prior to establishing the optimal products (Fernando et al., 2006; Gosling, 2005; Harper and Gani, 2000). Wahlund et. al. (2004) systematically investigated several bioenergy processing alternatives to quantify the specific cost of CO₂ emissions

reduction of each method. The method attempts to discover which method brings about the greatest CO₂ reduction at the lowest cost. A case study in Sweden showed that biomass was best utilized as a pelletized coal substitute. Huber and Corma (2007) propose utilizing existing infrastructure and oil refineries to process biomass into higher valued chemicals and fuels through catalytic cracking and hydrotreating with more advanced catalysts. Because these unit operations are used widely in the petro-chemical industry their performance is understood and the equipment is already in place a more rapid transition to biofuels could result.

Cameron et. al. (2007) stated that the selection of an optimally sized biorefinery was a function of plant capital cost and distance variable costs for feedstock transport. Plant capacity did not depend upon harvesting, loading, or other distance fixed costs. Estimates of distance variable costs and distance fixed costs can also be insightful for making informed decisions regarding plant technology selection. Searcy and Flynn (2009) considered the tradeoff between larger capacity bio-processing facilities that reduce per unit production cost at the expense of greater delivered feedstock cost because of increasing required transportation. The trade-off between these two costs can be used to help select an optimally sized bio-processing facility. Thorsell et. al. (2004) performed techno-economic analysis to determine the optimal capacity and the harvesting cost incurred for a gasification-fermentation based biorefinery focusing specifically on harvesting technologies and equipment.

Lambert and Middleton (2010) sought to identify optimal harvest, storage, transportation, pretreatment, and refining activities for a cellulosic ethanol biofuel

production facility. A techno-economic analysis yielded marginal results at current price points for feedstock and product ethanol. Mapemba et. al. (2008) asserts that the harvest cost for biomass is not a fixed cost per unit as many modelers assume because of non-optimal work scheduling and unforeseeable weather constraints. An integer program is proposed that seeks to determine the optimal number of harvesting equipment accounting for the variable harvesting cost. In practice they found that endogenous models underestimate the number of required harvesters and the average cost per unit harvested. Hess et. al. (2007) developed scenarios to help study cellulosic ethanol production to identify important cost barriers and supply chain network improvements to address each barrier and ultimately achieve targeted price points for profitably ethanol production.

3.2 Biorefinery Supply Chain Optimization

With respect to the supply chain optimization for bio-refineries, van Dyken et al (2010) developed a mixed integer linear programming (MILP) model for the optimization of biomass supply chains by considering the effect on biomass quality of each step in transport, storage and processing where the primary biomass quality observed was the moisture and energy content. Dansereau et al. (2009) developed a margins-centric approach to the optimization of the forest-biorefinery supply chains. Mansoornejad et. al. (2010) developed a systematic methodology integrating the product and process selection with the supply chain design for a more robust decision making framework to optimize a forest biorefinery. Hess et. al. (2007) developed scenarios to help study cellulosic ethanol production to identify important cost barriers and supply

chain network improvements to address each barrier and ultimately achieve targeted price points for profitably ethanol production. Guillen et. al. (2005) derived a mathematical formulation combining a scheduling model with a cash flow and budgeting formulation for multi-product chemical supply chains and found that the integrated approach outperformed the traditional sequential method. Gigler et al. (2002) proposed a dynamic modeling approach towards optimization of agricultural or biomass supply chains, where the appearance and biomass quality were the two key parameters optimized; the appearance states are affected by handling and biomass quality is affected by processing, storage and transportation. Freppaz (2004) developed an optimization formulation considering the sales of energy produced, plant construction maintenance costs, biomass transportation and harvesting, energy distribution costs for decision support in determining the optimal amount of woody biomass to be used for energy production instead of other competing uses. Another study found that 39% of the energy content in wood pellets was used in transport for a case study involving the shipment of wood pellets from Vancouver, British Columbia to Stockholm, Sweden. The study recommended that wood pellets are used locally to reduce this value, and that wood residues should be used in place of natural gas during pellet formation and drying (Magelli et. al., 2009). Ravula et. al. (2008) compared biomass transportation strategies to determine an optimal method for the delivery of a weekly supply of feedstock to a biorefinery using trucks. A MILP was developed by Shastri et. al. (2009) for harvesting, packing, storage, biomass handling and transportation with the goal of optimizing feedstock procurement of a distributed seasonally available biomass. The model

considered both long term decisions like facility selection and mode of transportation and also shorter term operational decisions like fleet scheduling. Singh et. al. (2010) developed a mathematic model to analyze the transport cost of biomass to a power plant using two modes of transportation and three forms of biomass. Preprocessed briquette biomass had the lowest unit transportation cost, and the unit transportation cost decreased with increasing distance.

Sokhansanj and Fenton (2006) presented a dynamic integrated framework that conducts a biomass supply analysis and logistics model of collection, storage, and transport operations for supplying corn stover to a biorefinery highlighting on seasonal weather conditions. Graham et al. (2000) used a system to quantitatively model the geographic variation of suppliers and feed production and transportation costs with environmental considerations to account for geographic differences in factors that affect supply of biomass to biorefinery facilities. Oak Ridge National Laboratory (ORNL) has shown data that increased yields in different seasons will cause price variability. In addition, The US National Agricultural Statistics Service (NASS) collected historical data on weekly progress of major crops showing the influence by growing seasons. An assessment method to determine the optimal logistics management of a distributed biomass resource was developed by Alfonso et. al. (2009) that considered the amount of available biomass, its quality and seasonal availability, optimal plant sizing and also a CO₂ emissions balance for each biomass. When applied to a region of interest a list of promising locations from a logistical point of view is developed.

More recently biorefinery supply chain optimization has been partnered with geographic information systems (GIS) in order to increase the decision making ability of models. In order to account for geographic differences in factors that affect supply of biomass to biorefinery facilities, Graham, et al. (2000) used a system to quantitatively model the geographic variation of suppliers with environmental considerations. Nardi et. al. (2007) developed an optimization routine to minimize the transportation cost of a supply chain network for grains in Argentina utilizing several feedstock origins, multiple transportation methods and various destinations utilizing GIS software to map resource availability and destination location and capacity that were already in place. Voivontas et. al. (2001) utilized GIS to estimate the potential for biomass based power production based on economically exploitable biomass. The technique considers first the theoretical biomass, then the available, technological and exploitable potential of the biomass with the electricity production cost as a prime metric for identifying potential sites for a power facility. Masera et. al. (2006) a GIS based wood-fuel integrated supply and demand mapping model with the goal of sustainability assessment for wood-fuel utilization policy decisions. Parker, et. al. (2010) developed a model for biorefinery location selection using GIS to account for biomass availability and optimized for total industry wide profits considering facility location and transportation costs. The model was used to develop a reasonable biofuel supply curve for the western United States. The model considered three modes of transportation; truck, rail and barge.

Ekşioğlu et. al. (2009) developed a model to coordinate long term supply chain decisions like facility location selection and short term decisions like the amount of

biomass processed and routing strategies. Huang et. al. (2010) proposed a model for strategic design of future bioethanol supply chains utilizing biowaste as feedstock with an emphasis on economic performance and additional infrastructure requirements. However distributed preprocessing of biomass to reduce transportation costs was not considered in these works. Cundiff et. al. (2009) proposed a system in which farmers use harvesting equipment to transport biomass to satellite storage locations (SSL) with year round transportation of biomass from SSL's to a centralized biorefinery. Economic analysis found that a larger number of smaller sized SSL's may be the optimal configuration of the supply chain network.

Mahmudi and Flynn (2006) analyzed transshipment economics from truck to rail for several biomass types and determined the minimum required rail distance for each biomass type in order to justify transshipment. In some cases the minimum rail distance exceeded the maximum biomass draw distance for an economically sized power plant using biomass feedstock. A model for ranking different biomass supply chain configurations considering delivered biomass cost, supplied biomass quality, emissions, energy input supply chain, and maturity of supply chain technologies was developed and found that rail transport followed by trucking seemed to be the best modes of transportation for a large scale biorefinery (Kumar et. al., 2006). A comparison of the use of pipelines to transport bio-oil versus truck based transportation highlighting greenhouse gas emissions from transport was investigated by Pootakham and Kumar (2010). The work considered both electricity produced from biomass and coal for pipeline transport, as expected the biomass derived option was more favorable with

respect to life cycle assessment. Comparing the relative cost of moving finished products or energy versus the cost of moving feedstock to processing was a method proposed by Searcy et. al. (2007) to determine if a biomass processing facility should be located at the biomass source or near the final user. In the case of electric power generation, it was found that the transportation costs throughout the life of the project justified building the generation plant near the biomass. Torrefaction, a thermal pretreatment step, combined with pelletization to create a dense energy carrier was investigated by Uslu et. al. (2008). Analysis of the energy required for transporting the energy pellets showed that torrefaction and pelletization had significant advantages over pyrolysis oil or standard energy pellets.

Richard (2010) rightly identifies the importance of distributed biomass processing and densification to increasing the feedstock supply range of a biorefinery to accommodate larger scale facilities, but did not propose an empirical method of evaluating at which point preprocessing becomes economically optimal.

4. LOCATION SCIENCE

Location science is a field addressed by operations research in which the optimal location of a new facility is determined with respect to cost, profit, distance, service time, market coverage or some other desired attribute (Horner, 2009). Since several criteria are evaluated in order to find the optimal location the problem is often a multiple-criteria decision making problem. Farahani (2010) lists common objectives when solving a location problem:

- Minimizing the total setup cost
- Minimizing the longest distance from the existing facilities
- Minimizing fixed cost
- Minimizing total annual operating cost
- Maximizing service
- Minimizing average time/ distance traveled
- Minimizing maximum time/ distance traveled
- Minimizing the number of located facilities
- Maximizing responsiveness

ReVelle, et. al. (2008) classifies typical location problems in one of four broad categories:

Analytical models that assume all demands are distributed uniformly throughout a service area, the cost of locating a facility is fixed and constant throughout the service area and transportation cost per unit per distance is a fixed value.

Continuous models allow facilities to be located anywhere within the service area with demands occurring at discrete points within the area. Demands are weighted on a

coordinate system and distances between demands are linear. The objective of these models is to minimize the overall demand weighted distance.

Network models place the location problem on a series of links and nodes with demand occurring at each node. Solutions typically involve developing special structures that yield polynomial time algorithms.

Discrete models assume a discrete set of demands and number of potential locations. Mixed integer linear programming is often used to solve discrete location problems.

When siting multiple locations the key variables are largely the same as when siting a single facility with the addition of variables that address the interdependencies of locations such as distance between facilities or the optimal number of facilities to be located (Griffith and Lea, 2005).

4.1 p-median Location Problem Formulation

ReVelle and Swain (1970) formulated the basic p-median facility location in which demands occur at each node and the objective function is to minimize the demand weighted total distances between demand nodes and the candidate facility locations.

$$\text{minimize } \sum_{j \in J} \sum_{i \in I} w_i d_{ij} y_{ij} \quad (1)$$

$$\sum_{j \in J} y_{ij} = 1 \quad \forall i \in I, \quad (2)$$

$$y_{ij} - x_j \leq 0 \quad \forall i \in I, \quad \forall j \in J, \quad (3)$$

$$\sum_{j \in J} x_j = p, \quad (4)$$

$$x_j \in \{0,1\} \quad \forall j \in J$$

$$y_{ij} \in \{0,1\} \quad \forall i \in I, \quad \forall j \in J$$

Where w_i is demand at node i , d_{ij} is the demand to destination distance, y_{ij} is the demand facility assignment integer, x_j is the facility location integer and p is the number of facilities.

The p-median problem assumes that the cost of locating a facility at each candidate site is equivalent. This is often not the case when selecting location for a large scale chemical processing facility. Access to adequate sources of fresh water, natural gas, electricity with sufficient land may reduce potential locations and constructing the facilities required to bring utilities into the plant may add significant fixed costs to a potential location. A simple extension to the above formulation can account for discrepancies between locations.

$$\text{minimize } \sum_{j \in J} f_j x_j \quad (5)$$

Where f_j is the anticipated location cost and the constraint $\sum_{j \in J} x_j = p$ has been relaxed as the use of facilities is penalized in the objective function.

4.2 Hub Location Science

Discrete hub location problems are one subset of location science of interest. Hubs are defined as facilities that serve as transshipment or switching points for transportation networks with multiple origins and destinations. Hubs also have application in electronic networks and data transfer such as telephone network design (Klincewicz, 1996). Studies on the hub location problems often assume three things: that the hub network is complete with a link between every hub pair; that there are economies of scale incorporated for using the inter-hub connections; and that no direct service (between two non-hub nodes) is allowed (Alumur and Kara, 2008). The objective of the hub location problem is to minimize the transportation cost of a unit from its point of origin to its final destination. There are several classifications of hub problems but the uncapacitated hub location problem is of particular interest. In the uncapacitated problem the number of hubs is unspecified but each hub has a predetermined fixed cost. Campbell (1994) outlined the different classes of discrete hub location problems and proposed integer programming techniques specific to each.

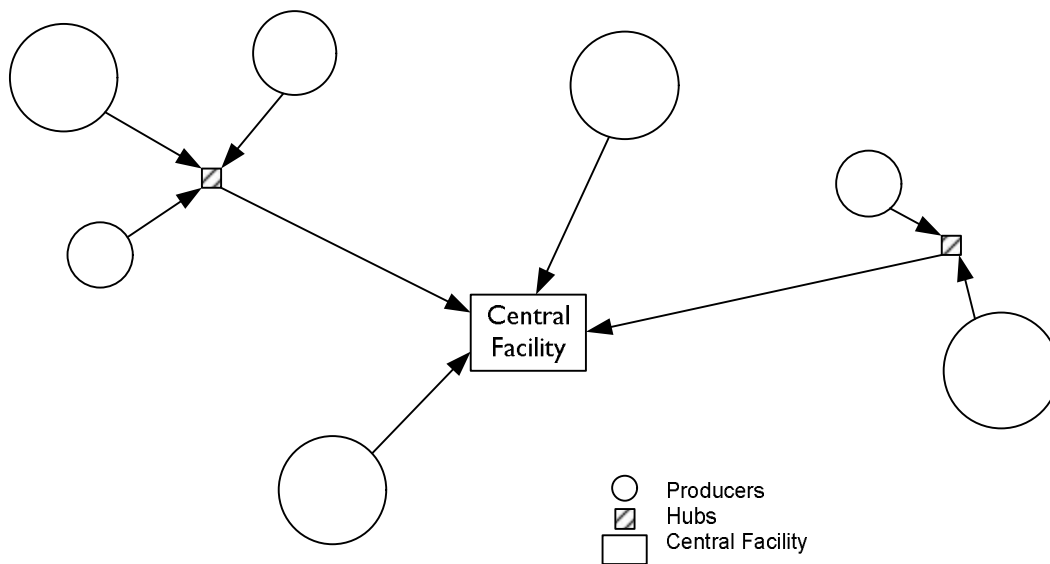


Figure 8. Distributed Processing Illustration

The use of hubs is of interest to the biofuels industry for their potential to preprocess biomass to a more valuable dense feedstock and reduce transportation costs.

With a better understanding of previous research in the area of biorefinery supply chain optimization and location selection two methodologies are proposed. The first is an optimization routine aimed at minimizing feedstock procurement and transportation cost for a biorefinery with multiple biomass sources available. This model also gives insight into scheduling when each biomass should be utilized and what technologies should be used for processing and the optimal size of the facility. The second problem is a formulation developed to determine the optimal configuration of a distributed biorefinery supply chain shown in Figure 8, based on transportation cost minimization, and whether distributed pre-processing hubs should be used to reduce operating cost.

5. TRANSPORTATION AND SCHEDULING PROBLEM

5.1 Problem Statement

It is desired to produce a certain amount of a given biofuel product in a centralized facility. Several biomass feedstocks may be used. Each feedstock, i , may be produced from various suppliers. Each supplier, j , can provide a given maximum supply of the feedstock that varies over time periods, k . The amounts shipped from each supplier to the central processing facility, the type and extent of processing pathways, and the scheduling of the transportation and processing are to be determined. The building blocks of the problem are shown by Figure 9. The boxes represent the variables that should be determined and the circles represent the parameters that are already known. The target is to find the minimum total cost for the system. The different cost items are described including feedstock cost, transportation cost, processing operating cost, and capital cost. These variables listed are dependent either on feedstock types i , producer locations j , available seasons k , processing facilities or combination of these. Constraints such as maximum capacity and feedstock yield are also included. The objective is to optimize this scheduling, transportation, and processing of feedstocks. GHG emissions are also included in the problem.

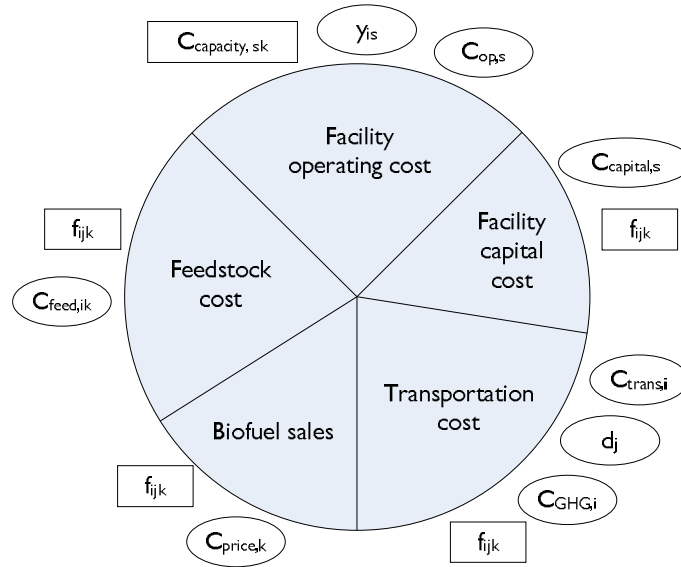


Figure 9. Schematic Representation of the Key Building Blocks of the Problem

5.2 Approach

For a given set of potential biomass feedstocks, the optimum processing techniques are to be determined and the optimum suppliers are to be selected. A hierarchical representation is developed to track the various pathways and species. In the first layer, the various suppliers are considered. Since each supplier may provide more than one feedstock, the second layer provides the selected feedstocks. The combination of supplier (j), feedstock (i), and time (k) determines the cost of biomass and the associated transportation cost and GHG emissions. Next, a processing layer is included where the processing costs and yields are taken into consideration. It is noted that not all the sections are chosen for each feedstock type. Therefore integers are

introduced to select the processing pathway for the selected feedstock from specific suppliers over certain time periods. Figure 10 is a schematic representation of the proposed structure.

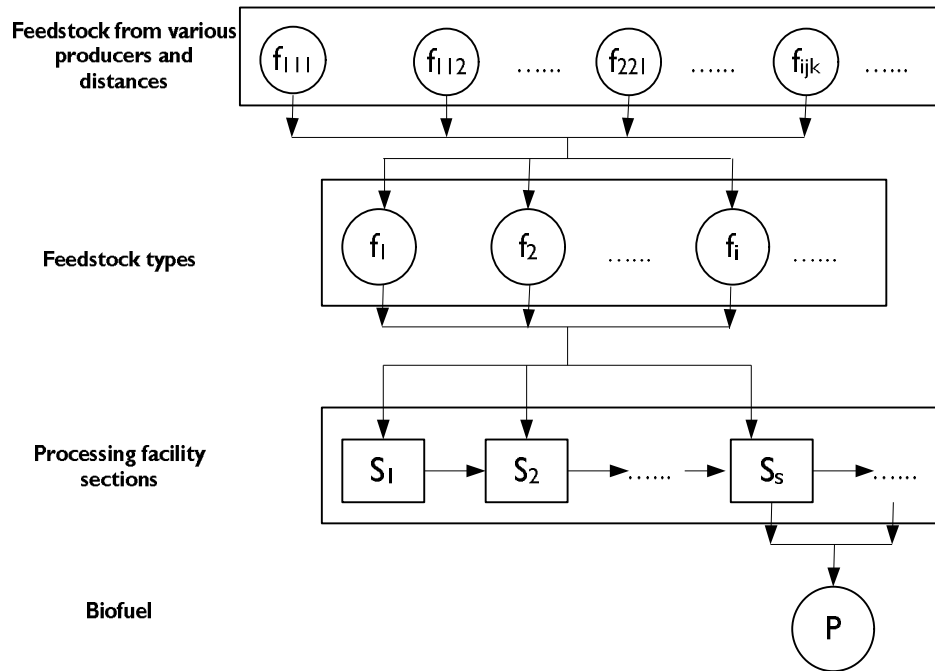


Figure 10. Structural Representation of the Approach

This can be achieved by developing an optimization routine centered on profit maximization in which producers are penalized for carbon emissions. The objective function will take the general form of:

$$\begin{aligned} \text{maxProfit} = & \text{sales} - \text{feedstock costs} - \text{operating costs} \\ & - \text{annualized capital costs} \end{aligned}$$

Each term in the previous equation will be described in greater detail in the following sections.

6. OBJECTIVE FUNCTION DEVELOPMENT

6.1 Feedstock Costs

Feedstock costs are broken down into four parts: the purchased feedstock cost, the transportation cost, the greenhouse gas emissions (GHG) associated with transportation, and the GHG emissions associated with the agriculture of the particular feedstock. The formulation makes use of four indexes i, j, k, s which correspond to feedstock type i , producer j , time period k and processing step s .

feed costs = cost of feedstock + transportation costs + GHG penalties

$$feed\ costs = \sum_{k=1}^K \sum_{j=1}^J \sum_{i=1}^I f_{ijk} * \{C_{ik}^{feed} + d_j * C_i^{trans} + d_j * C_i^{GHG,t} \mp C_i^{GHG,ag}\} \quad (6)$$

Table 1. Feedstock Cost Parameter Descriptions

Variable/Parameter	Description	Units
f_{ijk}	Incoming feed rate	mass/time
C_{ik}^{feed}	Cost of individual feed	USD/mass
C_i^{trans}	Transportation cost	USD/(mass*distance)
$C_i^{GHG,t}$	Carbon penalty, transportation	USD/(mass*distance)
$C_i^{GHG,ag}$	Carbon penalty/credit agriculture	USD/mass
d_j	Distance feed transported	distance

Table 2. Formulation Index Description

Index	Significance
i	Feedstock Type
j	Producer
k	Time Period

6.2 Sales

Product sales rate is found by the production of the facility and the market price for the final product. The production rate is found by the incoming feed rate and the entire process yield which is comprised of the product of the individual pathway section yields encountered by the particular feedstock. The pathway utilized for each particular feedstock type must be known in advance in order to determine the feedstock specific overall process yield.

$$sales = \sum_{k=1}^K \sum_{j=1}^J \sum_{i=1}^I f_{ijk} * y_i * C_k^{price} \quad (7)$$

$$y_i = \prod_{s=1}^S y_{s,i} \quad \forall i \quad (8)$$

Table 3. Sales Parameter Description

Variable/Parameter	Description	Units
f_{ijk}	Incoming feed rate	mass/time
y_i	Total Pathway yield	-
y_s	Plant section yield for feed i	-
C_k^{price}	Product market value	USD/volume

6.3 Operating Costs

The operating costs will be a function of the process feed rate and the feedstock selection as different feedstocks require different levels of processing. The overall processing cost for each feedstock can be broken down into the sum of the operating costs for each section of the plant encountered by a specific feedstock. Again, the process pathway for a given feedstock must be known in advance in order to determine this value.

$$operating\ costs = \sum_{i,j,k} f_{ijk} * C_i^{op} \quad (9)$$

$$C_i^{op} = \sum_{s=1}^S C_{s,i}^{op} * C_{si}^{capacity} \quad \forall i y_i = \prod_{s=1}^S y_{s,i} \quad \forall i \quad (10)$$

Table 4. Operating Cost Parameter Description

Variable/Parameter	Description	Units
f_{ijk}	Incoming feed rate	mass/time
C_i^{op}	Pathway operating cost factor	USD/mass
C_s^{op}	Section operating cost factor	USD/mass
$C_{si}^{capacity}$	Integer routing biomass	-

6.4 Capital Costs

Annualized capital costs are given by the summation of the cost associated with the largest capacity selected for each section normalized by the anticipated life of the project. Monthly production rates may dip below the upper bound of the maximum constructed capacity, but the annualized cost will be billed at the maximum size regardless of throughput for a particular time period. The maximum capacity through each section is determined by the initial maximum throughput of feedstock multiplied by the previous section yields. The maximum capacity of the plant is also limited to the maximum amount of biomass available for processing from each producer during each time period.

$$capital\ costs = \sum_{s=1}^S \frac{C_s^{capacity} * C_s^{capital}}{l} \quad (11)$$

$$C_{sk}^{capacity} = \sum_{i=1}^I \left(C_{si}^{capacity} * f_{ijk} * \prod_{1}^{s-1} y_{s,i} \right) \forall s, k \quad (12)$$

$$C_{sk}^{capacity} \leq C_s^{capacity} \quad \forall s f_{ijk} \leq f_{ijk}^{max} \quad \forall i, j, k \quad (13)$$

Table 5. Capital Cost Parameter Description

Variable/Parameter	Description	Units
$C_s^{capacity}$	Total capacity of section	mass/time
$C_s^{capital}$	Capital cost rate of section	USD/mass
$C_{sk}^{capacity}$	Utilized capacity of section during period	mass/time
$C_{si}^{capacity}$	Integer routing feedstock i through section s	Binary integer
f_{ijk}	Incoming feed rate	mass/time
y_s	Plant section yield	-
l	Plant lifetime	time

7. SCHEDULING CASE STUDIES

7.1 Scenario I

Biodiesel is to be produced from three potential feedstocks. Figures 11 and 12 provide the availability and cost data for the three feedstock types. Type 1 is a feedstock at low cost requiring greater processing. Type 2 is a higher-cost feedstock requiring fewer processing steps. Type 3 feedstock is available year round with a consistent and expensive purchase cost requiring the fewest processing steps. Biomass is produced by four independent producers with facilities located at varying distances from the processing plant as given by Table 6.

Table 6. Distances from the Producers to the Centralized Facility

Producer	Biomass Type	Distance (miles)
1	Type 3	5
2	Type 3	15
3	Type 1 and 2	20
4	Type 1 and 2	25

Each biomass has unique characteristics that require different levels of processing to convert to the biofuel product. Biomass specific yields (ton desired product/ton species processed by technology section) for each section of the plant are shown in Table 7 along with the operating cost in USD per ton processed for each biomass through each required section of the plant. Biomass specific transport costs in USD/distance are also shown.

Table 7. Yields, Operating Cost (\$/ton), and Transportation Cost

Biomass Type	Technology Section 1		Technology Section 2		Technology Section 3		Transport Cost (USD/ton mile)
	Yield / $C_{s,i}^{op}$		Yield / $C_{s,i}^{op}$		Yield / $C_{s,i}^{op}$		
1	0.98	20	0.80	10	0.85	24	0.13
2	1	-	0.75	12	0.80	25	0.23
3	1	-	1	-	0.85	26	0.23

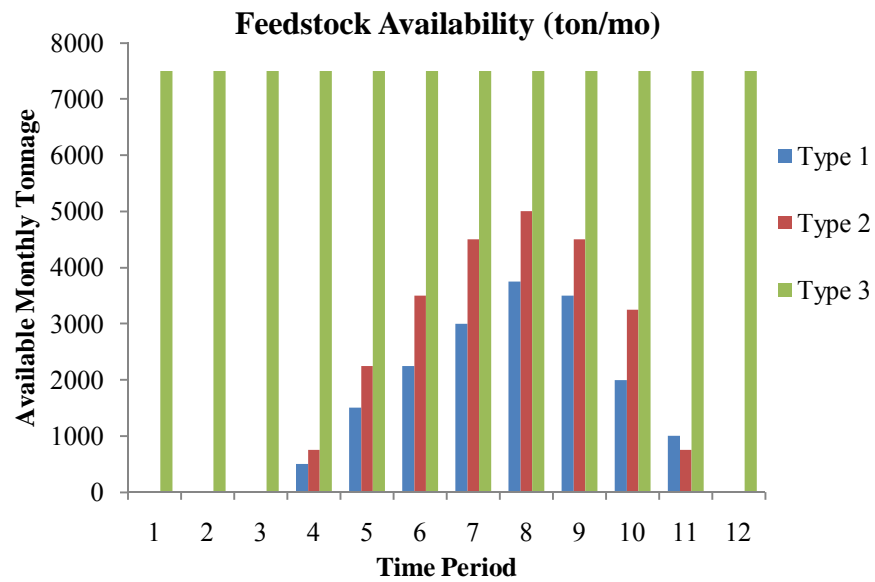


Figure 11. Data on Feedstock Availability for Scenario I

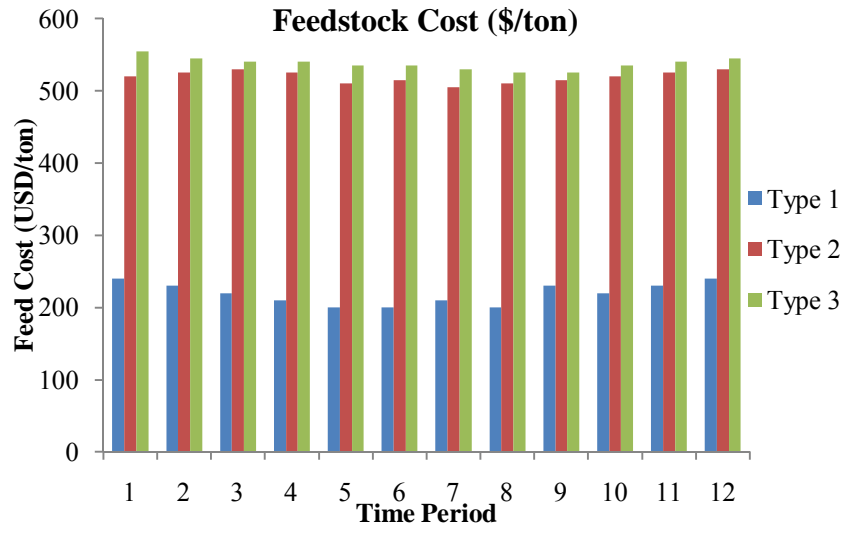


Figure 12. Data on Feedstock Price for Scenario I

The optimization results for Scenario 1 are summarized by Figure 13. The solution determines to process all available feedstocks I and III throughout the year while processing feedstock II in one month only.

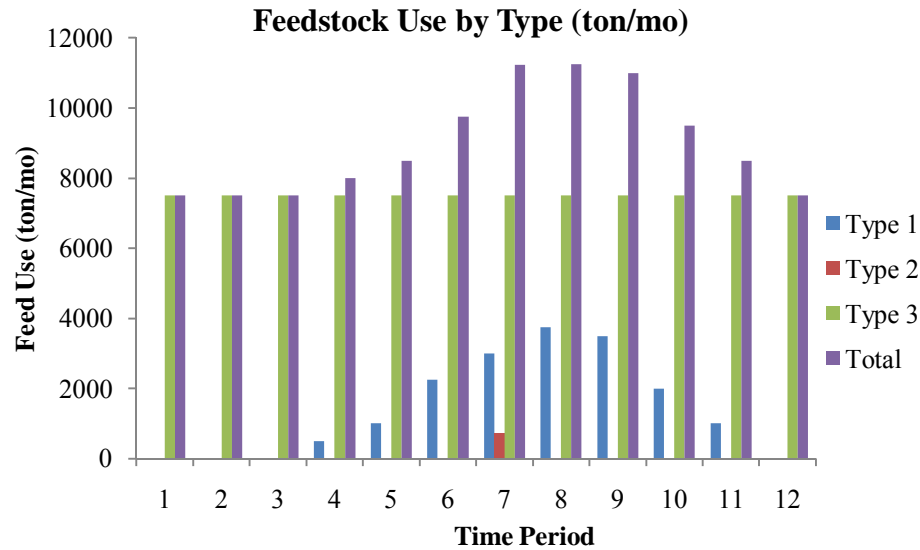


Figure 13. Results for Scenario I

7.2 Scenario II

Two feedstocks with offset harvest seasons are available; Type 1 with stable low price Type 2 with decreasing price during the harvest season. One feedstock available year round with a consistent and expensive purchasing cost requiring the fewest processing steps. Producer 4 that provides Feeds 1 and 2 has been moved to a location further from the centralized processing facility to illustrate the effect of producer distance on the results. This scenario attempts to model a producer who has two seed oil sources available with offset harvest seasons. The cheapest source has a stable price while the more expensive one experiences a dip in price during harvest which would be the case if the feedstock was considered to be perishable or expensive to store beyond harvest. The third feedstock available is again meant to represent a constantly available

more expensive feed source. The data for the three feedstocks are summarized by Figures 14 and 15.

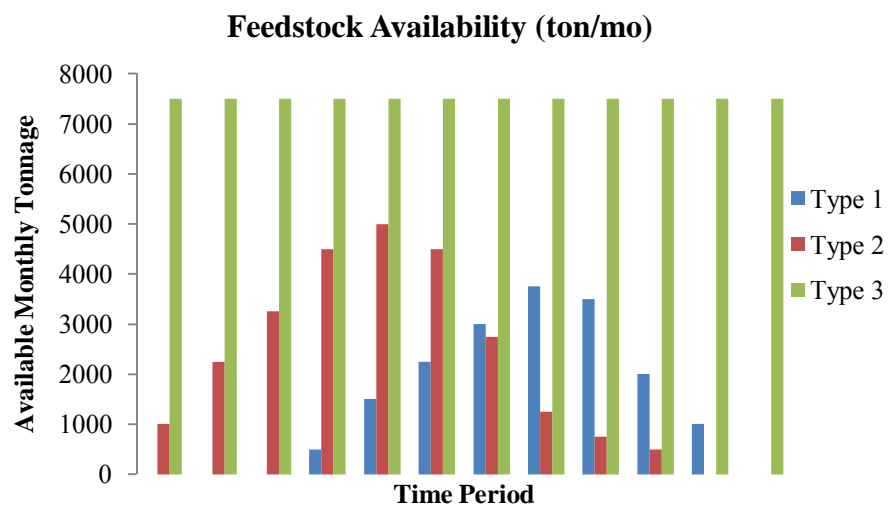


Figure 14. Data on Feedstocks Availability for Scenario II

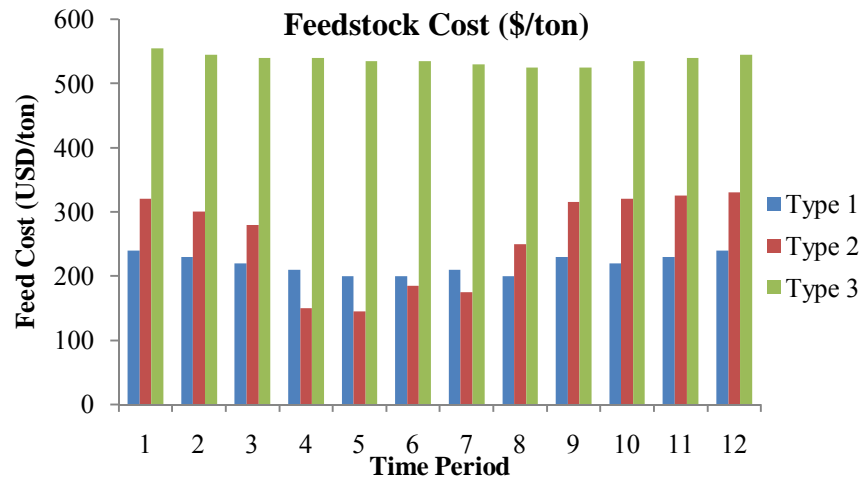


Figure 15. Data on Feedstock Cost for Scenario II

The results for Scenario II are shown by Figure 16. The model sensitivity to changes in distance (miles) from the producer of Type II feedstock to the processing facility is shown in Figure 17. The distance of producer two from the centralized facility was increased to show the effect on the amount of feedstock purchased from the particular producer. This effect can be made more pronounced by increasing the cost of transportation or the feedstock purchase price. The willingness to transport feedstock is also affected by the product sales price.

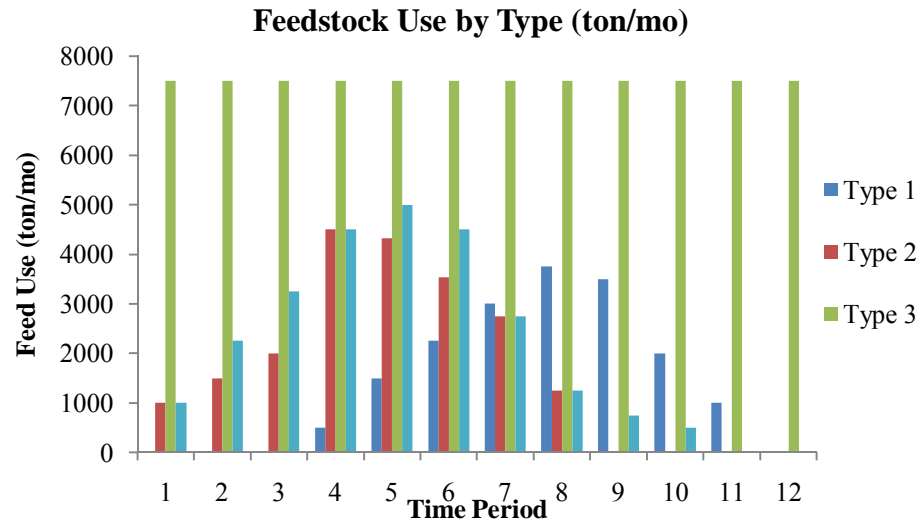


Figure 16. Summary of Solution Results for Scenario II

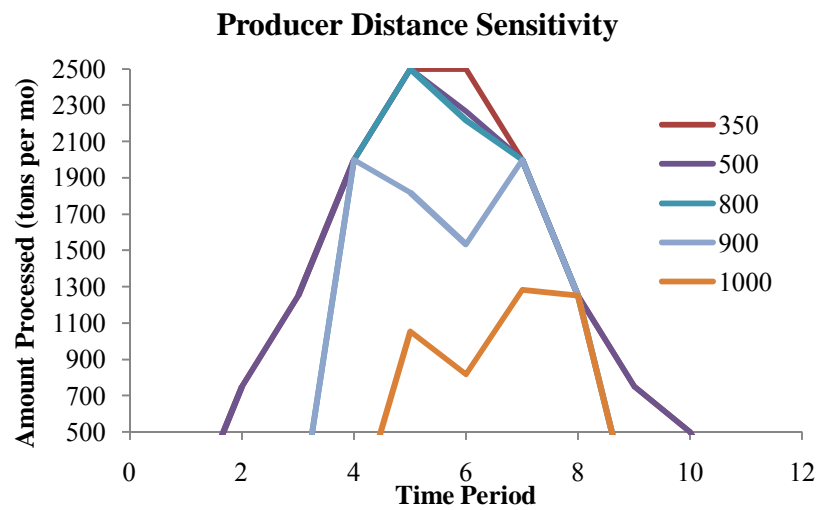


Figure 17. Distance Sensitivity Analysis

7.3 Scenario III

This scenario involves two feedstocks with distinct harvest seasons; Type 1 with a jump in price late in the year and Type 2 with a price dip corresponding to the peak harvest season. One feedstock is available year round with a consistent and expensive purchasing cost requiring the fewest processing steps. The data are summarized in Figures 18 and 19.

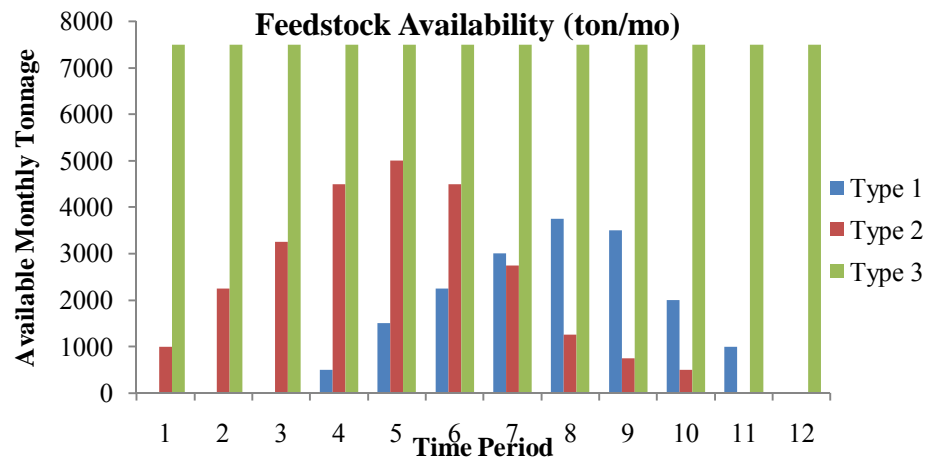


Figure 18. Feedstock Availability for Scenario III

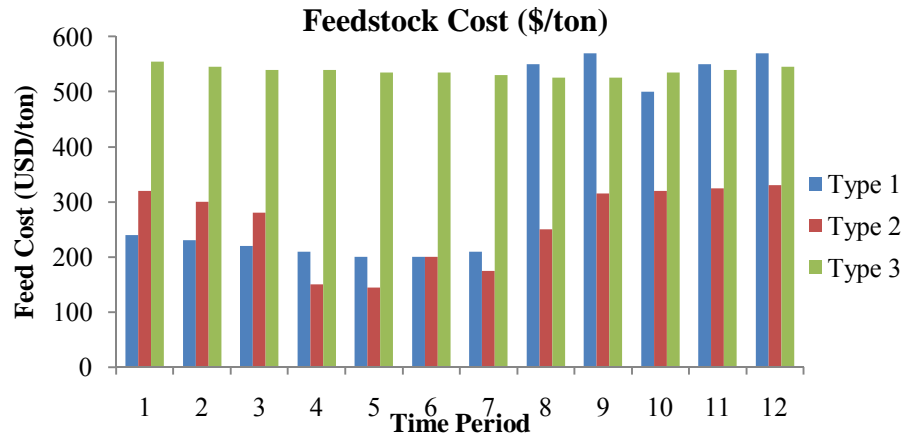


Figure 19. Feedstock Cost for Scenario III

The solution for Scenario III (Figure 20) indicate that it is optimal to process all available Type 2 and Type 3 biomass. Processing of Type 1 biomass is curtailed as prices increase. The model results show preference for Type 1 producer with closer proximity to the processing facility.

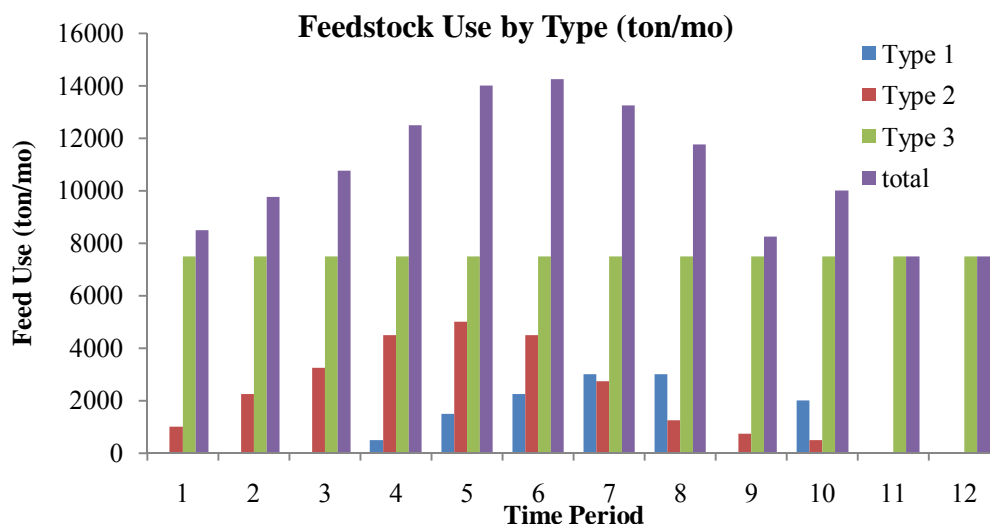


Figure 20. Summary of Results for Scenario III

7.4 Salient Points

In this formulation, a systematic procedure has been developed for the optimization of scheduling, transportation, and processing of biomass to biofuels. The developed model is an MILP which can be solved globally to provide useful insight for process designers. When given the appropriate information regarding feedstock availability and process performance parameters, the model can be readily used in sizing and scheduling a production facility. The model can also be used to identify crucial price points on the feedstock and product prices at which production should be curtailed or halted.

8. PREPROCESSING HUB AND FACILITY LOCATION PROBLEM

8.1 Problem Statement

Next is a formulation for providing insight into the optimization of distributed biorefineries. Given are a set of sources for the biomass feedstocks, a set of locations available to install preprocessing hub facilities, and a set of locations to install the central processing and distribution facilities. There are limits for the supply of the bioresources and for the demand for the products and subproducts. The problem is aimed at determining the optimal configuration for the processing and distribution system to yield the solution with the maximum total net profit considering the sales for the products and the cost for the raw materials, the transportation costs and the operating and capital costs for the facilities.

8.2 Model Formulation

Prior to the model formulation, the main indexes are defined. i corresponds to the agricultural areas where the feed is produced, j is an index to indicate the possible locations to install the hub preprocessing facilities, k indicates the locations able to install the centralized processing facilities, and l represents an index for the products and subproducts; finally, n , m and q are indexes for the disjunctions to determine the capital costs for the hub and central facilities.

The model formulation is based on the superstructure shown in Figure 21. It is worth noting here that the location process (see Figure 8) in this case is modeled as a source/interception/sink mass-integration representation (El-Halwagi, 2006). The

sources can send the bioresources to the preprocessing hubs or/and to the centralized biorefineries. After the preprocessing hubs process the bioresource, they produce an intermediate product that can be sent to the central facilities for further processing and subproducts that may be sold at that location. The final product is sent to consumers from the central facilities. The existence of the facilities (hubs and central facilities) is an optimization variable that must be determined.

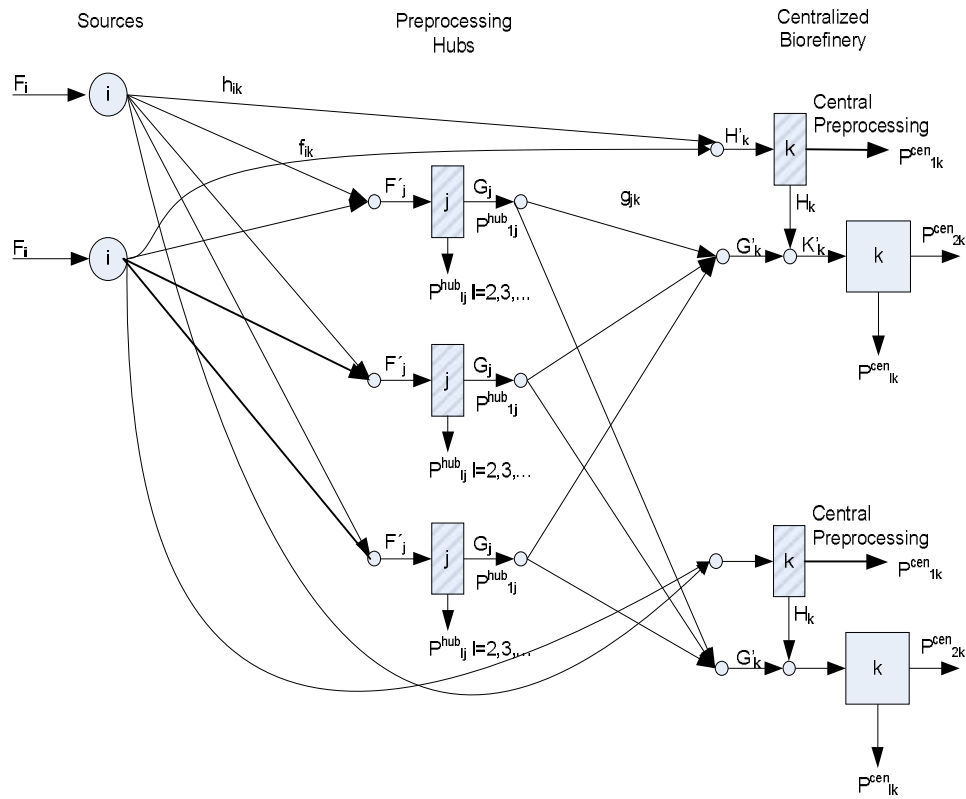


Figure 21. Superstructure for the model

The model must determine the network configuration and the optimal flowrates to yield the process with the maximum profit. Then, the model formulation is stated as follows.

8.2.1 Feedstock Supply Constraint

The total feedstock purchased from producer i (F_i) must be less than the total feedstock available from that producer (F_i^{max}), leading to the following constraint.

$$F_i \leq F_i^{max}, \quad \forall i \in I \quad (14)$$

8.2.3 Supply Feedstock Balances

Feedstock purchased from each producer i (F_i) may be routed to the nearest preprocessing hub j if this is selected via f_{ij} , or it may bypass the hub and ship directly to the preprocessing section of the centralized facility k via h_{ik} . This yields the next constraint.

$$F_i = \sum_j^J f_{ij} + \sum_k^K h_{ik}, \quad \forall i \in I \quad (15)$$

The amount of material entering the hubs and central facility from each producer must be equal to the purchased amount.

8.2.4 Material Balances Prior to the Hubs

The total material processed by each hub is defined as F'_j and this must be equal to the sum of the material from any feedstock i (f_{ij}).

$$F'_j = \sum_i^I f_{ij} \quad \forall j \in J \quad (16)$$

8.2.5 Hubs Processing Balances

The primary product at each hub ($l=1$) is passed on as the feed to the centralized processing facility so it is removed from the product slate via G_j in a manner that maintains model flexibility to sell intermediate products at hubs should this become the optimal business strategy.

$$P_{lj}^{hub} = \alpha_{lj}^{hub} F'_j - G_j \quad \forall l = 1, \quad \forall j \in J \quad (17)$$

For products other than the main ($l>1$) such as meal, heat and power, the co-products may be sold directly from the hub, and the material balance is stated as follows:

$$P_{lj}^{hub} = \alpha_{lj}^{hub} F'_j \quad \forall l > 1, \quad \forall j \in J \quad (18)$$

Here, α_{lj}^{hub} is the process yield per input for each product or co-product l at each hub j . If a hub is not designed with the ability to leverage a particular co-product, its yield is set as zero for that facility.

8.2.6 Mass Balance for the Inlet to the Central Processing

The feed to the central processing facility remains segregated in two categories, material that has passed through the hubs and has been through the preprocessing step G'_k and material transported directly to the central facility H'_k that still requires the intermediate processing step before conversion to biodiesel.

$$G'_k = \sum_j^J g_{jk} \quad \forall k \in K \quad (19)$$

$$H'_k = \sum_i^I h_{ik} \quad \forall k \in K \quad (20)$$

8.2.7 Balances for the Central Facilities Processing

The formation of products is also treated differently at the central processing facility since products from the preprocessing step may be passed on to the final processing step or sold as intermediate products at the central site. Therefore, we have the following equation for the main product:

$$P_{lk}^{cen} = \alpha_{lk}^{cen} H'_k - H_k \quad \forall l = 1, \quad \forall k \in K \quad (21)$$

And for the by-products:

$$P_{lk}^{cen} = \alpha_{lk}^{cen} K'_k \quad \forall l > 1, \quad \forall k \in K \quad (22)$$

The demand at each distribution point is valued by a commodity price specific to each location and is limited by a maximum demand constraint.

$$P_{lk}^{cen} < P_{lk}^{cenMAX} \quad \forall l \in L, \quad \forall k \in K \quad (23)$$

$$P_{lj}^{hub} < P_{lj}^{hubMAX} \quad \forall l \in L, \quad \forall j \in j \quad (24)$$

8.3 Objective Function

The objective function seeks to maximize profits while accounting for product sales, feedstock cost, transportation cost, preprocessing hub location assignment, central

facility location assignment and other operating costs. The general format of the objective function is stated as follows:

$$\begin{aligned} \text{Profits} = & \text{Product Sales} - \text{Feedstock Cost} - \text{Transportion Costs} - \\ & \text{Facility Capital Cost} - \text{Variable Operating Costs} \end{aligned}$$

Each section of the objective function is explained further in the sections below.

8.3.1 Product Sales

Vegetable oil, biodiesel, meal, syngas, heat and power may be produced in the central and hub facilities as intermediate, final or co-products. To account for production of a varied product slate at multiple potential locations the following formulation is used:

$$\text{Product Sales} = \sum_k^K \sum_l^L C_{lk}^{\text{cenprod}} P_{lk}^{\text{cen}} + \sum_j^J \sum_l^L C_{jl}^{\text{hubprod}} P_{lj}^{\text{hub}} \quad (25)$$

P_{lk}^{cen} and P_{lj}^{hub} are the amount either mass, MMBtu or kW of product l formed at central facility location k or at hub location j that is valued at C_{lk}^{cenprod} and C_{jl}^{hubprod} . It is worth noticing here that both the centralized and the hub facilities are able to produce final products and subproducts.

8.3.2 Feedstock Cost

The cost of feedstock used is simply the sum of the amount of feedstock purchased from each supplier i (F_i) plus any oil, if available, purchased by the centralized biodiesel plant k , K_k . C_i^{biomass} and C_k^{oil} are the prices of feedstock and fresh oil purchased, respectively. Then, the feedstock cost is calculated as follows:

$$Feedstock\ Cost = \sum_i^I F_i C_i^{biomass} + \sum_k^K K_k C_k^{oil} \quad (26)$$

8.3.3 Transportation Cost

The transportation cost is the sum of costs for transporting raw feedstock to preprocessing hubs or directly to the centralized facility and the cost of transporting oil from hubs to the centralized facility. f_{ij} , g_{jk} and h_{ik} are the amount of mass moved from producer to hub, hub to central and producer direct to central, respectively. C_{ij}^{trans} , C_{jk}^{trans} and C_{ik}^{trans} are the freight cost per ton per mile. Freight costs are function of the mode of transportation used; trucks, rail or barges may be used to move materials along the supply chain each with a different cost per ton per distance. Hub to central transportation is generally less expensive as the mode of transportation is more developed. In reducing the transportation costs, the optimization routine seeks to reduce the total weighted distance between all facilities. Then, the total transportation cost is stated as follows:

$$Transportation\ Cost = \sum_i^I \sum_j^J f_{ij} C_{ij}^{trans} + \sum_j^J \sum_k^K g_{jk} C_{jk}^{trans} + \sum_i^I \sum_k^K h_{ik} C_{ik}^{trans} \quad (27)$$

8.3.4 Facility Capital Cost

Next, the capital cost of locating a central facility or preprocessing hub must be considered otherwise the model would seek to build a facility at every candidate location

to reduce the transportation costs. Capital cost for each hub j , preprocessing central facility k , and central facility k can be calculated as follows:

$$\text{Facility Capital Costs} = \frac{[\sum_j^J \text{Cost}_j^{\text{hub}} + \sum_k^K \text{Cost}_k^{\text{cenPrep}} + \sum_k^K \text{Cost}_k^{\text{cen}}]}{\text{lifetime}} \quad (28)$$

The capital cost of a facility is assumed to be most heavily dependent upon the size of the facility. Potential locations with varying access to utilities or different needs specific to a location may also cause variability in location costs. It is worth noticing that usually the capital costs for the facilities follows a relationship of exponential capacity-ratio with exponent (i.e., $\text{Cost} = A + B(\text{Capacity})^c$, where A and B depend upon the type of facility and c is an exponent to account for scaling economies usually between 0.6 and 0.7). In addition, these facilities are restricted by a given maximum capacity, when this maximum capacity is overloaded an additional unit must be installed. A disjunctive formulation is used to linearize capital cost versus facility capacity curves. Figure 22 shows a schematic representation of the capital costs functions linearized. The preprocessing hub is used as an example.

The primary function of the preprocessing hub is to extract vegetable oil from the feedstock oil seeds likely using hexane solvent extraction techniques. Modular packaged units of fixed total capacity are available to perform this task with potentially multiple units located at one site to meet capacity requirements, and an example of the disjunction used for hub capital cost is shown next.

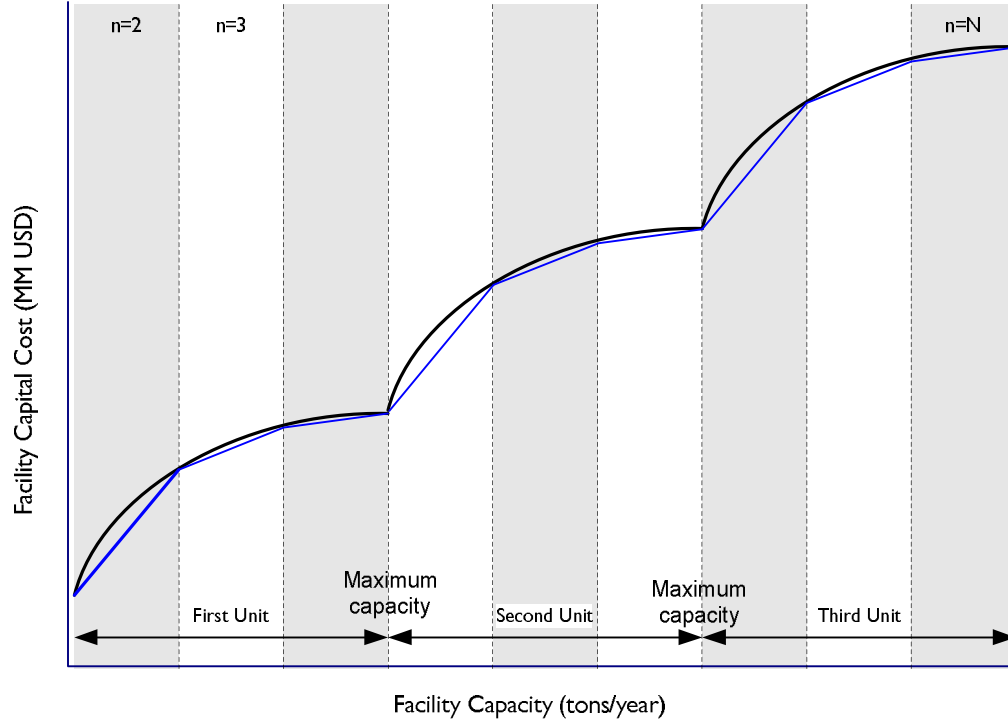


Figure 22. Linearized Facility Capital Cost Function

8.3.5 Capital Cost for Preprocessing Hubs Facilities

$$\forall n \in N \quad \forall j \in J \quad \left[\begin{array}{l} Y_{jn} \\ F'_{jn}{}^{min} \leq F'_j \leq F'_{jn}{}^{max} \\ Cost_j^{hub} = a_{jn} + b_{jn}F'_j \end{array} \right]$$

The previous disjunction states that the linear equation to determine the capital cost for the hubs depends on the capacity (as it was noted in Figure 22). Therefore, when

a given capacity is selected, the corresponding capital cost equation is selected. To model the previous disjunction, the following relationships are used.

First, only one disjunctive term can be selected, and this is modeled as follows,

$$\sum_n^N y_{jn} = 1, \quad \forall j \in J \quad (29)$$

The continuous variables are disaggregated as follows,

$$F'_j = \sum_n^N f'_{jn}, \quad \forall j \in J \quad (30)$$

$$Cost_j^{hub} = \sum_n^N C_{jn}^{hub}, \quad \forall j \in J \quad (31)$$

Then, the constraints inside the disjunctions are stated in terms of the disaggregated variables,

$$f_{jn}^{min} * y_{jn} \leq f'_{jn} \leq f_{jn}^{max} * y_{jn}, \quad \forall j \in J, \quad \forall n \in N \quad (32)$$

$$C_{jn}^{hub} = a_{jn} y_{jn} + b_{jn} f'_{jn}, \quad \forall j \in J, \quad \forall n \in N \quad (33)$$

Finally, upper and lower limits are imposed for the disaggregated variables,

$$C_{jn}^{hub} \leq C_j^{hubMAX} y_{jn}, \quad \forall j \in J, \quad \forall n \in N \quad (34)$$

$$f'_{jn} \geq 0, \quad \forall j \in J, \quad \forall n \in N \quad (35)$$

$$C_{jn}^{hub} \geq 0, \quad \forall j \in J, \quad \forall n \in N \quad (36)$$

To explain the previous relationships we have the following. When a segment of the disjunctive terms is selected, then the associated Boolean variable Y_{jn} is true and the associated binary variable y_{jn} must be equal to one. For all other cases, the Boolean and binary variables are false and zero, respectively; then, since the upper limits given by equations (32) and (34) for the segments not selected, the associated continuous disaggregated variables are zero, and the variables that are able to have values larger than zero are the ones for the disjunctive term selected. For equations (30) and (31) the continuous variables are equal to the disaggregated variables for the disjunctive term selected and the relationships are stated in terms of these disaggregated variables by relationships (32) and (33).

This same method is used to determine the capital cost of each facility. Cost curves are modified to reflect differences in location suitability or land costs. The total capital cost is then annualized throughout the expected lifetime of the project.

8.3.6 Capital Cost for Preprocessing Central Facilities

$$\forall q \in Q \left[\begin{array}{c} X_{kq} \\ H'_{kq}{}^{min} \leq H'_k \leq H'_{kq}{}^{max} \\ Cost_k^{cenPrep} = c_{kq} + d_{kq}H'_k \end{array} \right], \quad k \in K$$

The disjunction to determine the capital cost for the preprocessing central facility is similar to the one for the hubs and it is modeled as follows:

Only one segment can be selected,

$$\sum_q^Q x_{kq} = 1, \quad \forall k \in K \quad (37)$$

The continuous variables are disaggregated as follows,

$$H'_k = \sum_q^Q h'_{kq}, \quad \forall k \in K \quad (38)$$

$$Cost_k^{cenPrep} = \sum_q^Q C_{kq}^{cenPrep}, \quad \forall k \in K \quad (39)$$

The constraints inside the disjunctions are stated in terms of the disaggregated variables,

$$H_{kq}^{min} * x_{kq} \leq h'_{kq} \leq H_{kq}^{max} * x_{kq}, \quad \forall k \in K, \quad \forall q \in Q \quad (40)$$

$$C_{kq}^{cenPrep} = c_{kq} x_{kq} + d_{kq} h'_{kq}, \quad \forall k \in K, \quad \forall q \in Q \quad (41)$$

Finally, upper and lower limits are imposed for the disaggregated variables,

$$C_{kq}^{cenPrep} \leq C_k^{cenPrepMAX} x_{kq}, \quad \forall k \in K, \quad \forall q \in Q \quad (42)$$

$$h'_{kq} \geq 0, \quad \forall k \in K, \quad \forall q \in Q \quad (43)$$

$$C_{kq}^{cenPrep} \geq 0, \quad \forall k \in K, \quad \forall q \in Q \quad (44)$$

The explanation of previous disjunction is similar to the one for the preprocessing hubs.

8.3.7 Capital Cost for Central Facilities

$$\forall m \in M \left[\begin{array}{c} Z_{km} \\ K'_{km} \leq K'_k \leq K'_{km} \\ Cost_k^{cen} = r_{km} + s_{km} K'_k \end{array} \right], \quad k \in K$$

The disjunction to determine the capital cost for the central facility is similar to the other facilities previously explained:

Only one segment can be selected,

$$\sum_m^M z_{km} = 1, \quad \forall k \in K \quad (45)$$

The continuous variables are disaggregated as follows,

$$K'_k = \sum_m^M k'_{km}, \quad \forall k \in K \quad (46)$$

$$Cost_k^{cen} = \sum_m^M C_{km}^{cen}, \quad \forall k \in K \quad (47)$$

The constraints inside the disjunctions are stated in terms of the disaggregated variables,

$$K_{km}^{min} * z_{km} \leq k'_{km} \leq K_{km}^{max} * z_{km}, \quad \forall k \in K, \quad \forall m \in M \quad (48)$$

$$C_{kqm}^{cen} = r_{km} z_{km} + s_{km} k'_{km}, \quad \forall k \in K, \quad \forall m \in M \quad (49)$$

Finally, upper and lower limits are imposed for the disaggregated variables,

$$C_{km}^{cen} \leq C_k^{cenMAX} z_{km}, \quad \forall k \in K, \quad \forall m \in M \quad (50)$$

$$k'_{km} \geq 0, \quad \forall k \in K, \quad \forall m \in M \quad (51)$$

$$C_{km}^{cen} \geq 0, \quad \forall k \in K, \quad \forall m \in M \quad (52)$$

The explanation of previous disjunction is similar to the one for the preprocessing hubs.

8.3.8 Operating Cost

The operating cost considers variable costs of operations including labor, supervision, utilities, maintenance, supplies, lab charges, royalties, catalyst, solvents, taxes and insuranceⁱ (Peters and Timmerhaus, 1991). As an approximation in this model it is assumed that all of these charges are directly linearly dependent upon production levels. F'_j , K'_k and H'_k are the plant inlet feed rates (see Figure 21). $Cost_j^{op}$, $Cost_k^{op}$ and $Cost_k^{op\ pre}$ are the operating cost charge in USD per mass processed at each facility; then, the total operating cost is given by,

$$\text{Operating cost} = \sum_j^J Cost_j^{op} F'_j + \sum_k^K Cost_k^{op} K'_k + \sum_k^K Cost_k^{op\ pre} H'_k \quad (53)$$

Estimates for the variable operating cost of biodiesel production range from roughly \$93 to \$111 per ton of oil processed (e.g., van Grepen, 2006; Carriquiry, 2007).

8.4 Remarks

The model formulation is an MILP problem; therefore, a global optimal solution is guaranteed. The model considers typical exponential capital cost behavior for the processing facilities. The superstructure considers simultaneously distributed and centralized configurations.

9. LOCATION CASE STUDIES

9.1 Scenario 1

For this example problem, the case study to determine the optimal location of hubs and central facilities for the biomass processing to yield biodiesel is considered to show the applicability of the proposed methodology. Several locations with specific bioresource availabilities are considered (in Figure 23 identified with a diamond), there are two locations to install the central facilities identified in Figure 23 with triangles and there are also two locations to install preprocessing hubs (identified with squares in Figure 23). Tables 8 and 9 show the distances and the unitary transportation costs between the different locations considered for this case.

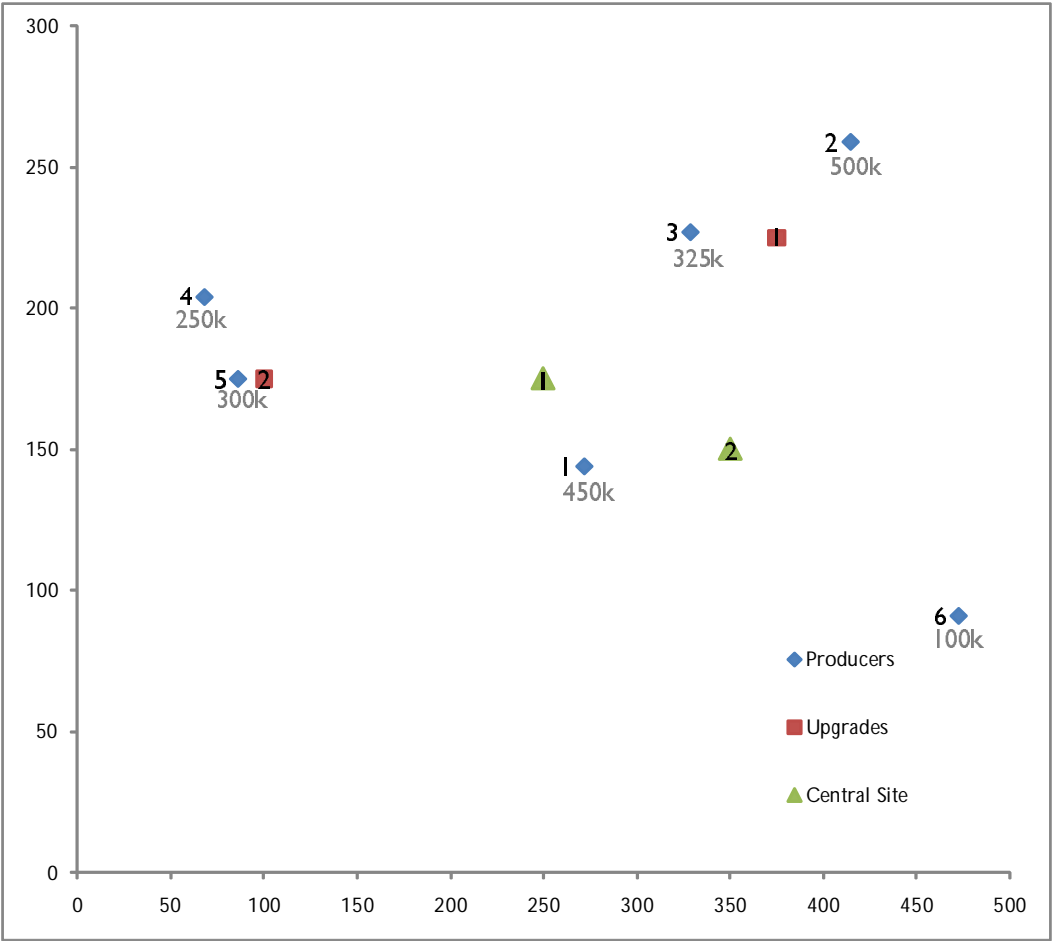


Figure 23. Map Configuration for the Case of Study

Table 8. Distances for Producers for the Case Study 1

Producers to hubs (miles)			Producers to centrals (miles)			Hubs to centrals (miles)		
Producer	Hub 1	Hub 2	Producer	Central 1	Central 2	Hub	Central 1	Central 2
1	131	175	1	38	78	1	135	150
2	52	326	2	185	127	2	79	251
3	46	235	3	95	80			
4	308	43	4	184	287			
5	293	14	5	164	265			
6	166	382	6	238	136			

Table 9. Transportation Costs for Case 1, (USD/ton)

Producers to hubs, C_{ij}^{trans}			Producers to centrals, C_{ik}^{trans}			Hubs to centrals, C_{jk}^{trans}		
Producer	Hub 1	Hub 2	Producer	Central 1	Central 2	Hub	Central 1	Central 2
1	13.10	17.48	1	1.90	3.91	1	5.39	6.00
2	5.25	32.60	2	9.26	6.35	2	3.16	10.05
3	4.60	23.48	3	4.73	3.99			
4	30.77	4.32	4	9.21	14.36			
5	29.33	1.40	5	8.20	13.26			
6	16.60	38.23	6	11.91	6.82			

Information regarding the cost of feedstock, intermediate and final products is shown in Table 10, and the process yields are shown in Table 11, these values were chosen to roughly correspond to an oil seed crop used to create FAME biodiesel. Much of the data used is best guess or order of magnitude estimates and should not be considered empirical.

Table 10. Commodity Pricing

Parameter	Description	Value (USD/ton)
$C_i^{biomass}$	Oil Seed Market Spot Price	Varied
C_k^{oil}	Vegetable Oil Spot Price	Not used
$C_{1k}^{cenprod}$	Vegetable Oil Contract Price	700
$C_{2k}^{cenprod}$	Meal Contract Price	250
$C_{3k}^{cenprod}$	Biodiesel Contract Price	800
$C_{1j}^{hubprod}$	Vegetable Oil Contract Price	700
$C_{2j}^{hubprod}$	Meal Contract Price	250
$C_{3j}^{hubprod}$	Biodiesel Contract Price	800

Table 11. Processing Yields

Parameter	Description	Value
α_{1j}^{hub}	Hub Oil Yield	0.18
α_{2j}^{hub}	Hub Meal Yield	0.82
α_{3j}^{hub}	Hub Biodiesel Yield	0
α_{1k}^{cen}	Central Oil Yield	0.20
α_{1k}^{cen}	Central Meal Yield	0.80
α_{3k}^{cen}	Central Biodiesel Yield	0.95
α_{4k}^{cen}	Central Waste Heat	0.14

Figure 24 shows the capital cost function for the preprocessing facilities, whereas Figures 25 and 26 show the capital cost function for the preprocessing and central facilities. Tables 12, 13 and 14 show the correlation data for these capital costs functions for hubs and central facilities, and the numbers used in the formulations are simply reasonable order of magnitude guesses to display the functionality of the model and should not be taken as accurate estimates of facilities capital costs.

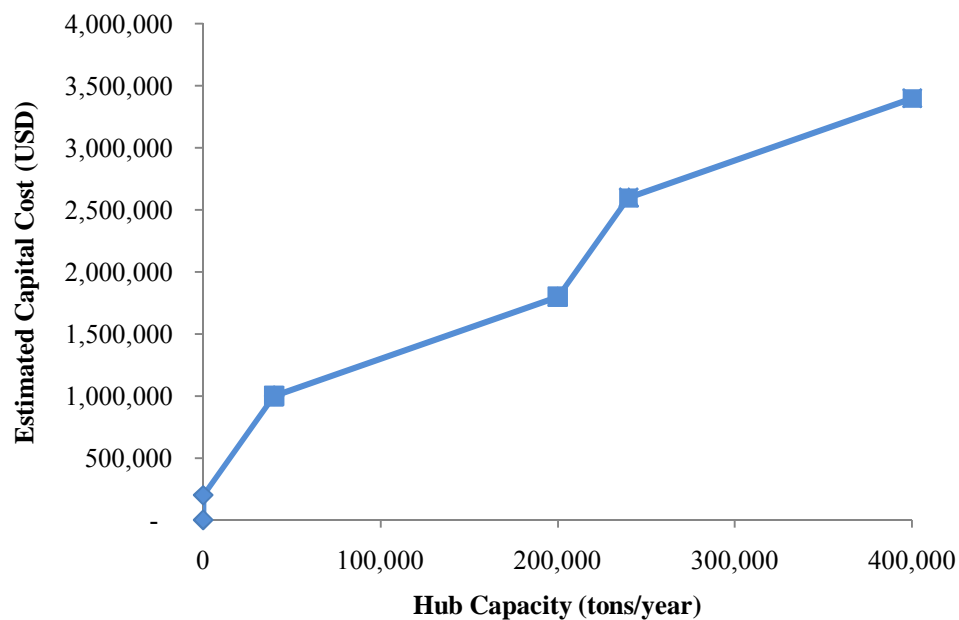


Figure 24. Capital Cost Function for the Preprocessing Facilities

Table 12. Data for Hub Disjunctive Relationships Capital Costs

Capacity Interval (tons/year)	a_{jn}	b_{jn}
0 – 40,000	200,000	20
40,001 – 200,000	800,000	5
200,001 – 240,000	-2,200,000	20
240,001 – 400,000	1,400,000	5

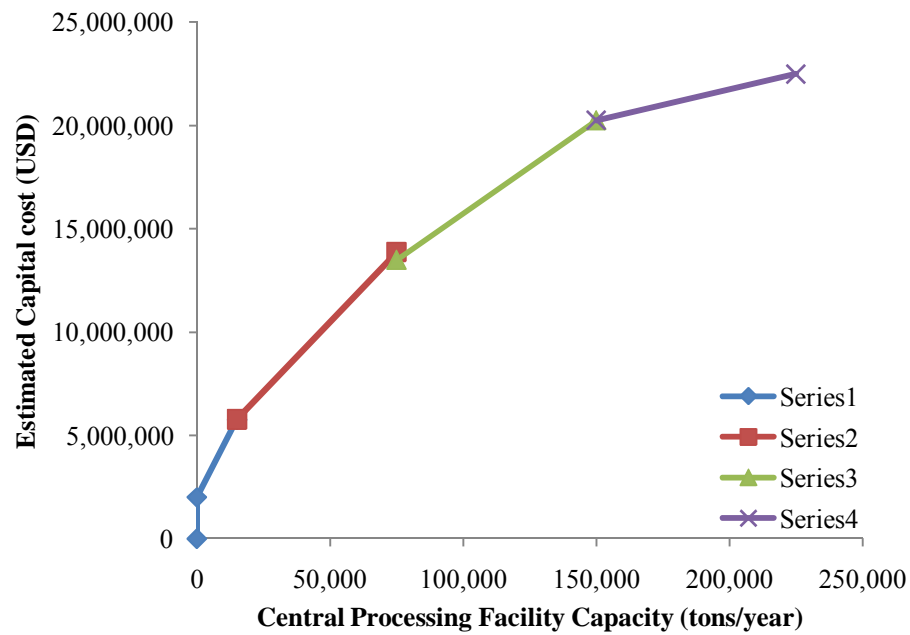


Figure 25. Capital Cost Function for the Central Processing Facility

Table 13. Central Processing Facility Capital Cost Data for Disjunctive Relationships

Capacity Interval (tons/year)	c_{km}	d_{km}
0 – 15,000	2,000,000	250
15,001 – 75,000	3,750,000	135
75,001 – 150,000	6,750,000	90
150,000 – 225,000	15,750,000	30

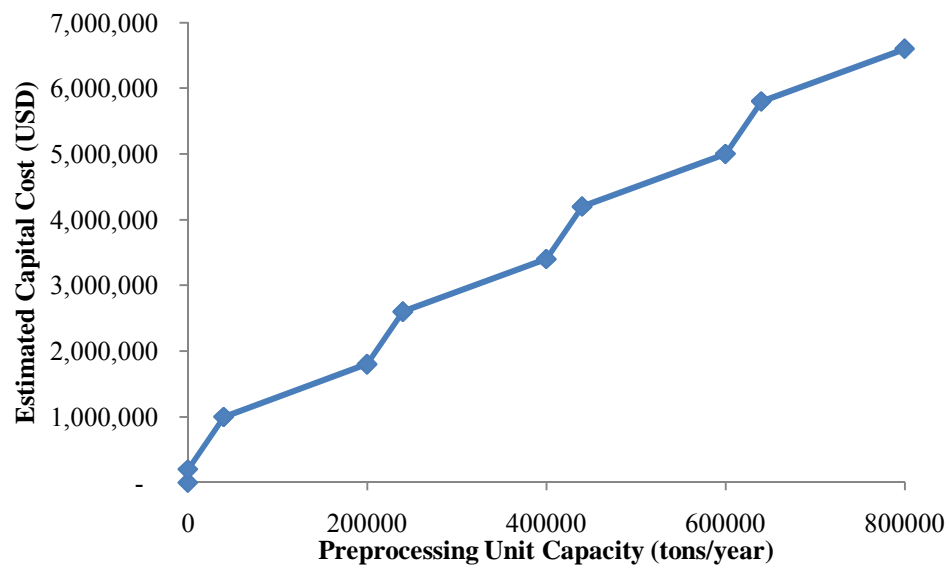


Figure 26. Capital Cost Function for the Centralized Preprocessing Unit

Table 14. Data for Central Preprocessing Units Capital Cost

Capacity Interval (tons/year)	r_{kq}	s_{kq}
0 – 40,000	200,000	20
40,001 – 200,000	800,000	5
200,001 – 240,000	-2,200,000	20
240,001 – 400,000	1,400,000	5
400,001 – 440,000	-4,600,000	20
440,001 – 600,000	2,000,000	5
600,001 – 640,000	-7,000,000	20
640,001 – 800,000	2,600,000	5

The problem then consists in determining the amount that each producer will send to each hub and central facility to yield the maximum overall profit reducing the overall transportation costs. The model consists of 38 binary variables, 219 continuous variables and 325 constraints to yield an MILP problem that was programmed in the software GAMS (Brooke et al., 2006) and it was solved in 0.09 sec of CPU time using an i7 at 2.67 GHz with 9 GB of RAM.

Table 15 shows the results for different cases analyzed for different scenarios for the feed price, this table also includes the capacities for each facility constructed in the network. It is worth noticing here that as feed prices rise, the annual profits decrease as modifications are made to the supply chain decreasing the scope of the operation reducing capital expenses and transportation costs. Table 15 also shows the results for

the case when the centralized solution is restricted to a single central processing facility. Notice that the distributed solution presents significant savings respect to the centralized solution for all scenarios for the feed price analyzed.

Table 15. Results for Case 1

Feed Price	Objective Value (USD/year)	Distributed solution (tons/year)				Centralized Solution (USD/year)
		Hub 1	Hub 2	Central 1	Central 2	
305	28,248,788		240,000	203,000	160,000	15,921,938
310	19,738,750			160,000	160,000	11,245,250
315	11,738,750			160,000	160,000	7,245,250
320	3,738,750			160,000	160,000	3,245,250
322	1,689,000			155,555		1,646,000
325	0					0

Table 16 shows the feedstock purchasing variation for case of study 1. The behavior obtained is explained as follows, as the price of the feed increases, preference is given to producers closer to the selected production facilities.

Table 16. Feedstock Purchase Quantities for Example 1, (tons/year)

Feed Price(USD)	305	310	315	320	322	325
Producer 1	4.50E+05	4.50E+05	4.50E+05	4.50E+05	4.50E+05	-
Producer 2	5.00E+05	5.00E+05	5.00E+05	5.00E+05	-	-
Producer 3	3.25E+05	3.25E+05	3.25E+05	3.25E+05	3.25E+05	-
Producer 4	1.65E+05	-	-	-	-	-
Producer 5	3.00E+05	2.25E+05	2.25E+05	2.25E+05	-	-
Producer 6	1.00E+05	1.00E+05	1.00E+05	1.00E+05	-	-

9.2 Scenario II

The distribution for the producers, hubs and central facilities are shown in Figure 27 for this case study. The distances and the transportation costs are shown in Tables 17 and 18, respectively.

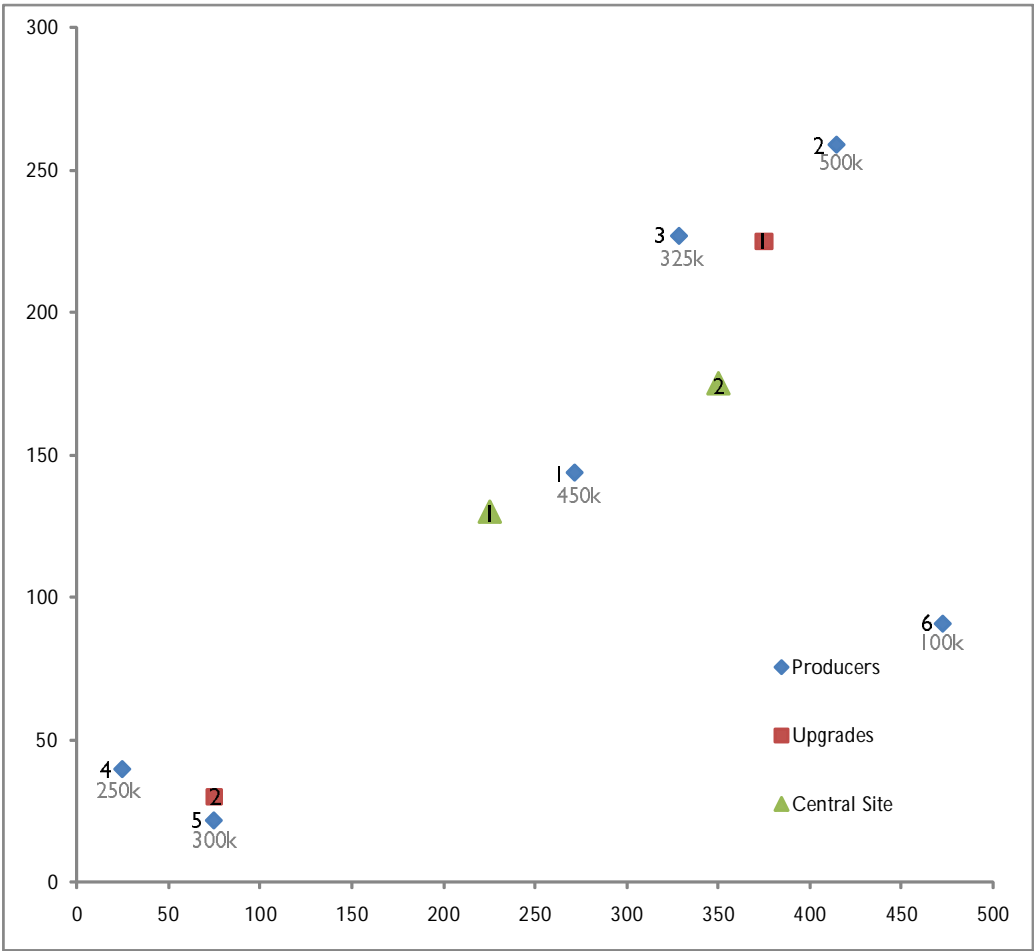


Figure 27. Resource Map for Case Study 2

Table 17. Distances for the Case Study 2, (miles)

Producers to hubs			Producers to central			Hubs to central		
Producer	Hub	Hub	Producer	Central	Central	Hub	Central	Central
1	131	228	1	49	84	1	178	180
2	52	410	2	230	106	2	56	311
3	46	321	3	142	56			
4	396	51	4	219	352			
5	362	8	5	185	315			
6	166	403	6	251	149			

Table 18. Transport Cost for Case Study 2, (USD/ton)

Producers to hubs, C_{ij}^{trans}			Producers to centrals, C_{ik}^{trans}			Hubs to centrals, C_{jk}^{trans}		
Prod	Hub 1	Hub 2	Prod	Central 1	Central 2	Hub	Central 1	Central 2
1	13.10	22.76	1	4.90	8.39	1	3.55	3.61
2	5.25	40.99	2	22.97	10.62	2	1.12	6.22
3	4.60	32.14	3	14.22	5.61			
4	39.59	5.10	4	21.93	35.19			
5	36.22	0.80	5	18.48	31.47			
6	16.60	40.26	6	25.10	14.89			

The same capital costs functions for the facilities used in the first case study are used in the second case study.

The proposed model consists of 219 continuous variables, 38 binary variables and 325 constraints. To analyze the results, several scenarios are proposed; this is, the price of feed was fixed but the transport costs were varied. The transport costs were modified by varying the dollar per ton per mile rate as follows it is shown in Table 19. For this case of study the feed cost was fixed as 305 \$/ton except the third scenario the feed prices from producers 4 and 5 were decreased to 295\$/ton. Table 20 shows the results for the different scenarios analyzed for the Example 2. Even though the configuration is the same for all scenarios, the material distributions are different. In

addition, the total profit for the centralized solution is always less than the distributed solution.

Table 19. Scenarios for the Transport Cost Factors for Example 2 (USD/ton mile)

Scenario	i to j	j to k	i to k
1	0.07	0.03	0.07
2	0.1	0.02	0.1
3	0.1	0.02	0.1

Table 20. Results for Case Study 2

Scenario	Distributed solution					Centralized solution
	Objective Value	Hub 1	Hub 2	Central 1	Central 2	
1	25,124,220		325,000	218,500	160,000	12,856,370
2	19,618,430		200,000	196,000	150,000	15,066,746
3	25,621,890		225,000	200,500	160,000	12,856,370

9.3 Conclusions

This section presents a mathematical programming model for the optimal placement of distributed biorefineries. The model includes the optimal selection of biomass from different sources, and the possibility to send it to preprocessing hubs facilities or send it directly to central processing and distribution facilities. The model is able to determine the amount of each material sent to each facility and the amount of

products and subproducts that must be produced for each facility to determine the maximum total net profit considering the transportation costs and the operating and capital costs for the facilities. The capital costs for the facilities consider the power-law behaviors that are modeled through a set of disjunctive formulations to linearize the model as a mixed integer linear programming problem to guarantee the global optimal solution of the problem. The application of the proposed methodology shows that the distributed configurations usually represent better solutions than the centralized solutions. No numerical complications were observed in the solutions of the examples analyzed.

10. CONCLUSION

This work presents two optimization formulations seeking to assist production planners in capital and operations decision making. The first formulation is useful for providing insight into feedstock scheduling and optimal facility sizing when utilizing a seasonally available biomass as feed. The model assists not only with feedstock scheduling but also can assist in technology selection and facility sizing if the appropriate data is available.

The next formulation provides a systematic method for decision making when considering distributed or centralized biorefining. The problem is solved as a geographically based source sink model. In addition to selecting the optimal between multiple purposed locations, this model also determines the best facility size considering the available biomass and the non-linear nature of facility capital cost.

Both formulations are presented in hopes that through application of systems optimization techniques to biorefinery supply chain decision making a more efficient system is designed leading to a more competitive, economically viable and attractive biofuel is the result.

NOMENCLATURE

*The following nomenclature is used in sections 5-7

i	Feedstock type
j	Producer
k	Time Period
f_{ijk}	Incoming feed rate
C_{ik}^{feed}	Cost of individual feed
C_i^{trans}	Transportation cost
$C_i^{GHG,t}$	Carbon penalty, transportation
$C_i^{GHG,ag}$	Carbon penalty/credit agriculture
d_j	Distance feed transported
y_i	Total Pathway yield
y_s	Plant section yield for feed i
C_k^{price}	Product market value
C_i^{op}	Pathway operating cost factor
C_s^{op}	Section operating cost factor
$C_{si}^{capacity}$	Integer routing biomass
$C_s^{capacity}$	Total capacity of section
$C_s^{capital}$	Capital cost rate of section
$C_{sk}^{capacity}$	Utilized capacity of section during period

l Plant lifetime

* The following nomenclature is used in sections 8-9

a_{jn}	Linearization constant
α_{lj}^{hub}	Hub product yields
α_{lk}^{cen}	Central product yields
b_{jn}	Linearization constant
c_{kn}	Linearization constant
$C_{lk}^{cenprod}$	Central product price
$C_{lj}^{hubprod}$	Hub product price
$C_i^{biomass}$	Feed price
C_k^{oil}	Make-up oil price
C_{ij}^{trans}	Producer to hub freight cost
C_{jk}^{trans}	Hub to central freight cost
C_{jn}^{hub}	Hub cost in linearized interval
C_{kn}^{cen}	Central cost in linearized interval
$C_{kq}^{cenprep}$	Central preprocessing cost in linearized interval
$Cost_j^{hub}$	Hub j capital cost
$Cost_k^{cen}$	Central k capital cost
$Cost_k^{cenPrep}$	Central preprocessing k capital cost
$Cost_j^{op}$	Hub operating cost

$Cost_k^{op}$	Central operating cost
C_j^{hubMAX}	Max cost of hub
C_k^{cenMAX}	Max cost of central
$C_k^{cenpreMAX}$	Max cost of central preprocessing section
d_{kn}	Linearization constant
F_i^{max}	Max supply constraint
F_i	Purchased feedstock
f_{ij}	Feedstock routed i to j
F'_j	Sum of feedstock into hub j
f'_{jn}	Hub feedrate in linearized interval
f_{jn}^{min}	Linearized interval minimum
f_{jn}^{max}	Linearized interval maximum
G_j	Intermediate leaving hub j
g_{jk}	Intermediate routed j to k
G'_k	Sum of intermediate into central k
h_{ik}	Feedstock routed i to k
H'_k	Sum of raw feed to central k
H_k	Processed feed leaving centralized preprocessing
h'_{kq}	Central preprocessing feedrate in linearized interval
h_{kq}^{min}	Linearized interval minimum
h_{kq}^{max}	Linearized interval maximum

K_k	Make-up oil
K'_k	Sum of intermediate and processed raw feed at k
k'_{kn}	Central feedrate in linearized interval
k_{kq}^{min}	Linearized interval minimum
k_{kq}^{max}	Linearized interval maximum
m_{kq}	Linearization constant
n_{kq}	Linearization constant
p_{lj}^{hub}	Product l leaving hub j
p_{lk}^{cen}	Product l leaving central k
p_{lj}^{hubMAX}	Maximum hub product demand
p_{lk}^{cenMAX}	Maximum central product demand
r_{km}	Linearization constant
s_{km}	Linearization constant
X_{kq}	Binary variable for interval selection
Y_{jn}	Binary variable for interval selection
Z_{km}	Binary variable for interval selection

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